



**Centurion**  
**UNIVERSITY**

*Shaping Lives...*  
*Empowering Communities...*

**Centurion University of Technology & Management**

**School of Applied Sciences**

**B.Sc. (Chemistry)**

**(Three years programme)**

**2020**

### CHOICE BASED CREDIT SYSTEM IN B.Sc. (Honours)

Semester	Basket-1	Basket-2	Basket -3	Basket-4	Basket-5	Semester wise cumulative credits
Semester	Core	Ability Enhancement	Domain	Discipline Specific Elective	Skill	
I	C 1	Environmental Science (02 Credit)	Domain Courses of Minimum 26 credits upto maximum of 36 credits.	G - 1	At least 04 skill courses of 16 credits	Minimum 24 Credits
	C 2					
II	C 3	JOB Readiness (English) (06 Credit)		G - 2		Minimum 24 Credits
	C 4					
III	C 5			G - 3		Minimum 24 Credits
	C 6					
	C 7					
IV	C 8			G - 4		Minimum 24 Credits
	C 9					
	C 10					
V	C 11					Minimum 24 Credits
	C 12					
VI	C 13					Minimum 24 Credits
	C 14					
<b>Total Credits</b>						<b>Minimum 140</b>
* A student can opt more number of <b>Domain /GE courses</b> up to a maximum of 20 credits over the period of six semesters						<b>Maximum 160</b>

**Department of Chemistry**

<b>Sl No</b>	<b>Course Code</b>	<b>Course Name</b>	<b>Credit</b>	<b>Type [T+Pr+Pj]</b>
1	CUTM1469	Atomic Structure and Chemical bonding-I	6	3+2+1
2	CUTM1470	States of matter and ionic equilibrium	6	3+2+1
3	CUTM1471	Basics and Hydrocarbons	6	3+2+1
4	CUTM1472	Chemical Thermodynamics and its application	6	3+2+1
5	CUTM1473	S- and P-block elements	6	3+2+1
6	CUTM1474	Oxygen Containing Functional Groups	6	3+2+1
7	CUTM1475	Phase Equilibria& Chemical Kinetics	6	3+2+1
8	CUTM1476	Coordination Chemistry	6	3+2+1
9	CUTM1477	Heterocyclic Chemistry	6	3+2+1
10	CUTM1478	Electrochemistry	6	3+2+1
11	CUTM1479	Bio-molecules	6	3+2+1
12	CUTM1480	Quantum Chemistry & Spectroscopy	6	3+2+1
13	CUTM1481	Organometallic chemistry	6	3+2+1
14	CUTM1482	Spectroscopy	6	3+2+1

### DOMAIN – RENEWABLE ENERGY

Sl. No	Code	Subject Name	Type of Courses	T-P-Pr(Credit)	Credits
1	CURE2190	Materials for Renewable Energy applications	Theory + Practice	(1-1-0)	2
2	CURE2191	Renewable Energy Technology for Industrial Process	Practice	1-2-0	3
3	CURE2192	Micro-grid Design & Implementation	Practice	0-2-0	2
4	CURE2193	Hybrid Renewable Energy Systems	Theory + Practice	1-2-0	4
5	CURE2194	Solar Off-grid Entrepreneur	Theory + Practice	1-1-0	4
6	CURE2195	Project	Practice	0-0-6	4
7	CURE2196	Internship	Practice	0-0-4	4

#### 1. Renewable Energy

#### Course Outline

Code	Course Title	T-P-Pj (Credit)	Prerequisite
CUTM1469	Atomic Structure and Bonding	3-2-1	

#### Objective

- To study and compare between various theories of atomic structure.
- To know the most common structure and hybridization observed for different compounds.
- To use periodic trend to understand the chemistry of alkali metals, alkaline earth metals, halogens, transition as well as inner transition elements.

### Course outcome

COs	Course outcomes	Mapping COs with POs (High-3, Medium-2, Low-1)
CO1	The student will acquire knowledge in the structure, bonding, and hybridisation of different compounds, their periodic properties and the quantum mechanical aspect.	PO1 (3)
CO2	Research and Problem Solving by Study and comparison between various theories of atomic structure and chemical bonding.	PO2(3)
CO3	Design and Development on improved experimental and theoretical knowledge by doing experiments	PO3(1)

### Course content

#### Module I

##### Atomic structure-I (10h)

Bohr's theory, its limitations and atomic spectrum of hydrogen atom, Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrodinger's wave equation, significance of  $\Psi$  and  $\Psi^2$ .

**Assignment-1:** Photoelectric Effect

**Assignment-2:** Sommerfeld Extension of the Bohr Theory

**Practice-1:** Determine the atomic configuration and bonding ability (Vlab)

**Practice-2:** Rutherford's gold foil experiments

#### Module II

### **Atomic structure-2 (12h)**

Quantum numbers and their significance, Normalized and orthogonal wave functions. Sign of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of s, p, d and f orbital's. Contour boundary and probability diagrams. Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations, Variation of orbital energy with atomic number.

**Assignment-3:** Atomic term symbol

**Practice-3:** Build an Atom (VLab)

**Practice-4:** Early experiment to characterize the atom

### **Module III**

#### **Periodic Properties-I (9h)**

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

**Assignment-4:** Application of effective nuclear charge

**Assignment-5:** Shielding effect of inner-shell electrons on the valence shell electron

**Practice-5:** The Periodic table of elements (Vlab)

### **Module IV**

#### **Periodic Properties-II (10h)**

Electron gain enthalpy, trends of electron gain enthalpy. Electronegativity, Pauling's/ Mulliken's electronegativity scales. Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity.

**Assignment-6:** Polarizing powder and Polarizability

**Practice-6:** Estimation of free alkali present in different soaps/detergents (Vlab)

**Practice-7:** Estimation of Barium (Vlab).

**Practice-8:** Estimation of Fe(II) and oxalic acid using standardized  $\text{KMnO}_4$  solution.

## Module V

### Chemical Bonding-I(Ionic Bonding) (7h)

Ionic bond: General characteristics, types of ions, size effects, radius ratio rule and its limitations, Packing of ions in crystals, Born-Landé equation Madelung constant, Born-Haber cycle and its application, solvation energy.

**Assignment -7:** Radius ratio of different cubic crystal structures

**Practice-9:** Determine the solubilities of solid compounds in water and in ethanol

## Module VI

### Chemical Bonding-II (Covalent Bonding-I) (9h)

Covalent bond: Lewis structure, Valence Bond theory (Heitler-London approach), Energetic of hybridization, equivalent and non-equivalent hybrid orbitals, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules, Formal charge, Valence shell electron pair repulsion theory (VSEPR).

**Assignment-8:** Wave mechanical treatment of covalent bond

**Practice-10:** Comparing ionic and Covalent compounds (Vlab)

**Practice-11:** Compare the melting points of various compounds.

## Module VII

### Chemical Bonding-III (Covalent Bonding-II) (9h)

Covalent character in ionic compounds, polarizing power and polarisability, 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

**Assignment-9:** Molecular orbital's for homonuclear diatomic molecules

**Assignment-10:** Term symbols for a diatomic molecule

**Practice-12:** Determine the conductivity of water solutions of the soluble solids

### Book References:



- Lee, J.D. Concise Inorganic Chemistry, ELBS, 1991.
- Douglas, B.E. and Mc Daniel, D.H., Concepts & Models of Inorganic Chemistry, Oxford, 1970
- Atkins, P.W. & Paula, J. Physical Chemistry, Oxford Press, 2006.
- Day, M.C. and Selbin, J. Theoretical Inorganic Chemistry, ACS Publications 1962.

### Course Outline

Code	Course Title	T-P-Pj (Credit)	Prerequisite
CUTM1470	States of Matter and Ionic Equilibrium	3-2-1	

#### Objective

- To develop basic and advance concepts regarding the three states of matter.
- To derive the expressions for determining the physical properties of gases, liquids and solids.

### Course Outcome

COs	Course outcomes	Mapping COs with POs (High-3, Medium-2, Low-1)
CO1	Knowledge on Derivation of mathematical expressions for different properties of gas, liquid and solids and understand their physical significance. Explain the crystal structure and calculate related properties of cubic systems.	PO1 (3)
CO2	Research and Problem Solving by Explaining the concept of ionization of electrolytes with emphasis on weak acid	PO2(3)



	and base and hydrolysis of salt.	
CO3	Design and Development by applying the concepts of gas equations, pH and electrolytes while studying other chemistry courses in everyday life and industries.	PO3(2), PO4 (1), PO5(1)

### Course content

#### Module I

##### Gaseous state-I (7h)

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

**Assignment-1:** Empirical Gas Laws

**Assignment-2:** Ideal gas equation

#### Module II

##### Gaseous state-II (8h)

Maxwell Boltzmann distribution laws of molecular velocities, Molecular energies (graphic representation – derivation not required) and their importance, Temperature dependence of these distributions. Most probable, average and root mean square velocities, Collision cross section, collision number, collision frequency, collision diameter and mean free path of molecules. Viscosity of gases and effect of temperature and pressure on coefficient of viscosity (qualitative treatment only)

**Assignment-3:** Degrees of freedom of the gaseous molecule

**Assignment-4:** Liquefaction of gases

#### Module III

##### Liquid state (13h)

Qualitative treatment of the structure of the liquid state, 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. Temperature variation of viscosity of liquids and comparison with that of gases

**Assignment-5:** Thermodynamic and intermolecular forces in solution

**Practice-1:** Determination of surface tension

**Practice-2:** Determination of Viscosity of Organic Solvents

**Practice-3:** Determination of co-efficient of viscosity of an unknown aqueous solution

**Practice-4:** Study the variation of surface tension of detergent solutions with concentration

## Module IV

### Solid state (7h)

Nature of the solid state, law of constancy of interfacial angles, law of rational indices, Miller indices, Elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices. X-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method, Analysis of powder diffraction patterns of NaCl, CsCl and KCl

**Assignment-6:** Calculating the intensity of diffraction using the structure factor equation

**Practice-5:** Indexing of a given powder diffraction pattern of a cubic crystalline system.

## Module V

### Ionic equilibria-I (10h)

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 ions effect, dissociation constants of mono and diprotic acids

**Assignment -7:** Strength of acids and bases

**Practice-6:** Determination of the pH scale by the method of successive dilutions

**Practice-7:** Study the effect of addition of HCl/NaOH on pH to the solutions of acetic acid, sodium acetate and their mixtures.

## Module VI

### Ionic equilibria-II (10h)

Degree of ionization, factors affecting degree of ionization, Ionization constant and ionic product of water, Buffer solutions; derivation of Henderson equation and its applications, Solubility and solubility product of sparingly soluble salts – applications of solubility product principle

**Assignment-8:** Mixture of two weak acids

**Assignment-9:** Ionization of polyprotic acids

**Practice-8:** Determination of solubility product

**Practice-9:** Designing a buffer solution with a specific pH

## Module VII

### Ionic equilibria-III (11h)

Qualitative treatment of acid – base titration curves, Calculation of pH at various stages, Theory of acid–base indicators, Selection of indicators and their limitations

**Assignment-10:** Common acid-base indicators and their properties

**Practice-10:** To determine the amount of substance in a solution of unknown concentration using various titrimetric methods

**Practice-11:** pH metric titration of (i) strong acid with strong base, (ii) weak acid with strong base

**Practice-12:** Determination of dissociation constant of a weak acid

### Book References:

#### Theory:

Atkins, P.W.; Paula, J.de. (2014),Atkin's Physical Chemistry Ed., 10th Edition, Oxford University Press.

Ball, D. W. (2017),Physical Chemistry, 2nd Edition,Cengage Learning, India.

Castellan, G. W. (2004),Physical Chemistry, 4th Edition, Narosa.

Kapoor, K.L. (2015), A Textbook of Physical Chemistry, Vol 1, 6th Edition, McGraw Hill Education.

Practical:

Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.

Kapoor, K.L. (2019), A Textbook of Physical Chemistry, Vol.7, 1st Edition, McGraw Hill Education.

Garland, C. W.; Nibler, J. W.; Shoemaker, D. P. (2003), Experiments in Physical Chemistry, 8th Edition, McGraw-Hill, New York.

### Additional Resources:

Moore, W.J. (1972), **Physical Chemistry**, 5th Edition, Longmans Green & Co. Ltd.

Glasstone, S. (1948), **Textbook of Physical Chemistry**, D. Van Nostrand company

## Course Outline

Code	Course Title	T-P-P (Credit)	Prerequisite
CUTM1471	Basics and Hydrocarbons	3-2-1	

### Objective

- The general concept of this course is to train students the fundamental laboratory skills like extraction, purification and separation techniques with some simple organic preparations.
- This helps students to gain experience to predict the functional group transformations, simple reaction mechanisms, and the synthesis of organic molecules by multi-step synthesis strategies

### Course outcome

COs	Course outcomes	Mapping COs with POs (High-3, Medium-2, Low-1)
CO1	Students will have a firm knowledge in the fundamentals and application of current chemical and scientific theories including those in Analytical, Inorganic, Organic and Physical Chemistries.	PO1 (3)
CO2	Research and Problem Solving by predicting the functional group	PO2(3)

	transformations, simple reaction mechanisms, and the synthesis of organic molecules by multi-step synthesis strategies	
CO3	Design and Development of scientific experiments as well as accurately record and analyze the results of such experiments.	PO3(2), PO4 (1)
CO4	Investigation, Judgment and communication to explore new areas of research in both chemistry and allied fields of science and technology.	PO3(2), PO5 (1), PO7(1)

### Course content

#### **Module -I: Basics of Organic Chemistry(5hrs)**

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.

**Practice-1** : Calibration of a Thermometer

**Assignment-1** : Organic Compounds, Electronic Displacements.

**Assignment-2** : Electronic Displacements, Organic acids and bases; their relative strength

#### **Module – II : Reaction Intermediate(4hrs)**

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.

**Practice-2** : Methods of purification of organic compounds.

**Assignment-3** : Reaction Intermediate

**Assignment-4 :** Introduction to types of organic reactions and their mechanism.

**Module – III : Chemistry of Aliphatic Hydrocarbons(2hrs)**

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

**Practice-3 :** Determination of the melting points of above compounds and unknown organic compounds (Kjeldahl method and electrically heated melting point)

**Practice-4 :** Effect of impurities on the melting point - mixed melting point of two unknown organic compounds.

**Module – IV : Carbon-Carbon pi bonds(8hrs)**

Formation of alkenes and alkynes by elimination reactions. Mechanism of E1, E2, E1cb reactions. Saytzeff and Hofmann eliminations. Reactions of alkenes: Electrophilic additions their mechanisms (Markownikoff/ Anti-Markownikoff addition). Mechanism of oxymercuration-demercuration, hydroboration-oxidation, ozonolysis, reduction (catalytic and chemical), syn and anti-hydroxylation (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.

**Practice-5 :** Determination of boiling point of liquid compounds. (boiling point lower than and more than 100 °C by distillation and capillary method)

**Practice-6 :** Separation of Amino acids by TLC

**Assignment-5 :** Elimination and Substitution reaction

**Assignment-6 :** Alkene, Reaction of Alkene

**Module – V : Aromatic Hydrocarbons(3hrs)**

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

**Practice-7 :** Detection of N,S, Cl, Br and I in organic compound.

**Practice-8 :** Test for Hydrocarbon.

**Assignment-7** : Reactions of alkynes, Aromaticity, Electrophilic aromatic substitution.

**Module - VI : Cycloalkanes and Conformational Analysis: (2hrs)**

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.

**Practice-9** : Preparation of Methane

**Practice-10** : Preparation of Ethene

**Assignment-8** : Cycloalkanes

**Module – VII : Stereochemistry(6hrs)**

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.

**Practice-11** : Preparation of Ethyne.

**Practice-12** : Preparation of cyclohexane from cyclohexanol.

**Assignment-9** : Conformation analysis of alkanes, Relative stability, Fischer Projection, Newmann and Sawhorse Projection formulae and their inter conversions .

**Assignment-10** : Stereochemistry.

**Text Books:**

1. University Chemistry, Vol. II, U.N Ojha and K.K Ojha, Himalaya Publishing House
- 2.Modern College Chemistry, Y.R Sharma and K.D Sharma, Kalyani Publishers

**Reference Books:**

- 1.Morrison, Boyd and Bhattacharjee, Organic Chemistry, 7<sup>th</sup> Edition, Pearson.
- 2.Kalsi, P. S. Stereochemistry Conformation and Mechanism, New Age International, 2005.



3. Eliel, E. L. & Wilen, S. H. Stereochemistry of Organic Compounds, Wiley: London, 1994.

### Course Outline.

Code	Course Title	T-P-Pj (Credit)	Prerequisite
CUTM1472	Chemical Thermodynamics and its Applications	(3-2-1)	

### Objective

- The Course covers the fundamentals laws of Thermodynamics and its related Phenomena
- To understand the applicability of chemical thermodynamics in various industrial processes as well as day to day life incidents.
- To understand the conceptual basis of thermodynamic scale of temperature as standard scale
- To understand the concept of chemical equilibrium in attaining high products by controlling various factors.
- To understand the concept of ideal and non-ideal solution along with various colligative properties.
- To practice various thermochemical experiments

### Course outcomes

COs	Course outcomes	Mapping COs with POs (High-3, Medium-2, Low-1)
CO1	Able to gain entire Knowledge on Thermodynamics, Chemical Equilibria and Colligative properties.	PO1 (3)
CO2	Research and Problem Solving of different thermodynamic equations, chemical equilibria and their relationship among each other.	PO2 (3), PO4 (2)
CO3	Design and Development by data interpretation and analysis for publication	PO3 (3)



## Course content

### **Module I : Introduction to Thermodynamics (6 hrs)**

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 condition, Calculations of q, w, U and H for irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions

### **Module II : Thermochemistry (12 hrs)**

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

**Practice 1:** 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).

**Practice 2:** Determination of heat capacity of the calorimeter and enthalpy of neutralization of hydrochloric acid with sodium hydroxide.

**Practice 3:** Determination of heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) solution of salts.

**Practice 4:** Determination of enthalpy of hydration of copper sulphate

### **Module III : Chemical Thermodynamics I (9 hrs)**

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; Free energy change and spontaneity, Relation between Joule-Thomson coefficient and other thermodynamic parameters; inversion temperature, Thermodynamic equation of state, Gibbs-Helmholtz equation, Maxwell relations

### **Module IV : Chemical Thermodynamics and Open System (5 hrs)**

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, Partial molar quantities

### **Module V : Chemical Equilibrium: I (10 hrs)**

Criteria of thermodynamic equilibrium, Degree of advancement of reaction, chemical equilibria in ideal gases, Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient, Concept of fugacity, Equilibrium constants and their quantitative dependence on temperature, pressure and concentration, Coupling of exoergic and endoergic reactions, Free energy of mixing and spontaneity

**Practice 5:** To study the shift of equilibrium between ferric ions and thiocyanate ions by increasing the concentration of either of them

### **Module VI : Chemical Equilibrium: II (8 hrs)**

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, Introduction to dilute Solutions, Introduction to Colligative Properties

**Practice 6 :** Le Chatelier principle in Contact Process (Demonstration)

**Practice 7 :** Le Chatelier principle in Haber Process (Demonstration)

### **Module VII: Colligative Properties (16 hrs)**

Excess thermodynamic functions, Thermodynamic derivation using chemical potential to derive relations between the relative lowering of vapour pressure and amount of solute, Raoult's and Henry's Laws and their applications, Thermodynamic derivation using chemical potential to derive relations between the elevation of boiling point and amount of solute, Thermodynamic derivation using chemical potential to derive relations between Depression of freezing point and amount of solute, Thermodynamic derivation using chemical potential to derive relations between the osmotic pressure and amount of solute, Applications in calculating molar masses of normal, dissociated and associated solutes in solution

**Practice 8:** To find the freezing point depression of a solution

**Practice 9:** To find the molar mass through freezing point depression of a solution

**Practice 10:** Determining the Vant Hoff's factor

**Practice 11:** To find the elevation of boiling point of a solution

**Practice 12:** To find the molar mass through elevation of boiling point of a solution

*Text Books:*

1. Atkins P. and De Paula, J. *Physical Chemistry Tenth Ed.*, OUP, 2014.
2. Castellan, G. W. *Physical Chemistry 4th Ed.*, Narosa, 2004.

*Reference Books:*

1. Engel, T. and Reid, P. *Physical Chemistry 3rd Ed.*, Prentice Hall, 2012
2. McQuarrie, D. A. and Simon, J. D. *Molecular Thermodynamics* Viva Books, 2004.
3. Roy, B. N. *Fundamentals of Classical and Statistical Thermodynamics* Wiley, 2001
4. Levine, I. N. *Physical Chemistry 6th Ed.* Tata Mc Graw Hill, 2010.

**Course Outline**

Code	Course Title	T-P-Pj (Credit)	Prerequisite
CUTM1473	<b>S and P block elements</b>	<b>3-2-1</b>	

**Objective**

- To identify the common physical properties of metals and non- metals and explain how their uses relate to these properties.
- To explore in depth specialized areas of chemistry of materials, including ores, metals, acids and bases and to understand how metals are extracted from their ores.
- To understand the trends in properties and reactivity of the s, p-block elements and noble gases.
- To become familiar with some of the roles of inorganic polymer and its applications in day to day life

**Course outcome**

COs	Course outcomes	Mapping COs with POs (High-3, Medium-2, Low-1)
CO1	Able to gain entire Knowledge on main group chemistry, including trends in	PO1 (3)

	oxidation states, periodic properties and complex formation tendency.	
CO2	Research and Problem Solving by identification of different main group element based nanostructure.	PO2 (3). PO4 (2)
CO3	Design and Development of the inorganic polymer-based material and interpret the data	PO3 (3), PO4 (2)

### Course content

#### **Module I (8 Hours )**

##### **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, Mond's process, Zone refining.

##### **Assignment-1**

##### **Practice-1**

Gravimetric Estimation of Barium

##### **Practice-2**

Crystallisation of copper sulphate

#### **Module II**

##### **Acids and Bases( 7 Hours)**

Bronsted-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.

##### **Assignment-2**

##### **Assignment-3**

### **Practice-3**

Preparation of Manganese (III) phosphate,  $\text{MnPO}_4 \cdot \text{H}_2\text{O}$ .

### **Practice-4**

Preparation of schiff base ligands

### **Module III( 8 Hours)**

#### **Chemistry of s and p Block Elements-1:**

Inert pair effect, Relative stability of different oxidation states, diagonal relationship, anomalous behaviour of first member of each group, Allotropy and catenation, Complex formation tendency of s and p block elements.

### **Assignment-4**

### **Practice-5**

Estimation of  $\text{Cu(II)}$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  using sodium thiosulphate solution iodometrically

### **Practice-6**

Synthesis of dibenzalacetone

### **Module IV( 9 Hours)**

#### **Chemistry of s and p Block Elements-2:**

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 nitrides, borohydrides (diborane).

### **Assignment-6**

### **Practice-7**

Preparation of potash alum,  $\text{K}_2\text{SO}_4 \cdot \text{Al}_2(\text{SO}_4)_3 \cdot 24\text{H}_2\text{O}$

### **Practice-8**

Analysis of Alloy (Brass)

### **Practice-9**

Synthesis of Schiff base metal complexes

### **Module V( 8 Hours)**

### **Chemistry of s and p Block Elements-3:**

Oxides and oxoacids of nitrogen, Phosphorus and chlorine, Peroxo acids of sulphur, interhalogen compounds, polyhalide ions, pseudohalogens and basic properties of halogens.

#### **Assignment-7**

#### **Assignment-8**

#### **Practice-10**

Estimation of available chlorine in bleaching powder

#### **Practice-11**

Gravimetric Estimation of Nickel

### **Module VI( 8 Hours)**

Noble Gases:

Occurrence and uses, rationalization of inertness of noble gases, Clathrates; preparation and properties of XeF<sub>2</sub>, XeF<sub>4</sub> and XeF<sub>6</sub>, Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF<sub>2</sub>), Molecular shapes of noble gas compounds (VSEPR theory).

#### **Assignment-9**

#### **Practice-12**

Preparation of Cuprous chloride, Cu<sub>2</sub>Cl<sub>2</sub>

### **Module VII( 8 Hours)**

Inorganic Polymers:

Types of inorganic polymers, comparison with organic polymers, synthesis, structural aspects and applications of silicones and siloxanes, Borazines, silicates, phosphazenes, and polysulphate.

#### **Assignment-10**

#### **Recommended Books:**

1. Lee, J.D. Concise Inorganic Chemistry, ELBS, 1991.
2. Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. Concepts & Models of Inorganic Chemistry 3rd Ed., John Wiley Sons, N.Y. 1994.

3. Greenwood, N.N. & Earnshaw. Chemistry of the Elements, Butterworth-Heinemann. 1997.
4. Cotton, F.A. & Wilkinson, G. Advanced Inorganic Chemistry, Wiley, VCH, 1999.
5. Rodger, G.E. Inorganic and Solid State Chemistry, Cengage Learning India Edition, 2002.
6. Miessler, G. L. & Donald, A. Tarr. Inorganic Chemistry 4th Ed., Pearson, 2010.
7. Atkin, P. Shriver & Atkins' Inorganic Chemistry 5th Ed. Oxford University Press (2010).
8. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009.

### Course Outline

Code	Course Title	T-P-Pj (Credit)	Prerequisite
CUTM1474	Oxygen Containing Functional Groups	3-2-1	

#### Objective

- The aim of this course to introduce basic practical skills to synthesize organic molecules containing functional groups like alcohols, acids, acid derivatives, carbonyl compounds, ethers, etc.
- In addition to that, the course will also help students to understand the reaction mechanism subjects in the later stages of their study.

#### Course outcome

COs	Course outcomes	Mapping COs with POs (High-3, Medium-2, Low-1)
CO1	Able to gain knowledge and understand the fundamentals of different organic molecules containing functional groups.	PO1 (3)
CO2	Research and Problem Solving on pharmaceutical chemistry and interpret the data for publication	PO2(3), PO3(2), PO4(1)
CO3	Design and Development of drug molecule used for different diseases.	PO3 (3), PO7(2)

## Course content

### **Module-1: Chemistry of Alkyl Halides**

Theory (4h)

- Alkyl halides: Methods of preparation of Alkyl halides
- Nucleophilic substitution Unimolecular (SN1) reaction
- Nucleophilic substitution Bimolecular (SN2) reaction and SNi mechanism
- Stereochemical aspects of SN1, SN2 and SNi reactions

Practice (2h)

- Functional group test for Alkyl halides

Assignment (2h)

- Nucleophilic substitution vs. Elimination.
- Effect of solvent on SN1, SN2 reaction mechanism

### **Module-2: Aryl Halides and Organometallic compounds**

Theory (4h)

- Preparation of Aryl halides including preparation from diazonium salts
- Nucleophilic aromatic substitution (SNAr) of aryl halides
- Benzyne mechanism
- Organometallic compounds of Mg and Li and use in the synthesis of organic compounds

Practice (4h)

- Preparation of benzene diazonium chloride.
- Synthesis of chlorobenzene from aniline

Assignment (2h)

- Relative reactivity of alkyl, allyl /benzyl, vinyl and aryl halides towards nucleophilic substitution reactions.
- Synthesis of organic compounds using organometallic compounds of Mg/Li.

### **Module-3: Alcohols**

Theory (4h)

- Preparation of Alcohols
- Properties and relative reactivity of 1°, 2°, 3° alcohols, Bouvaelt-Blanc Reduction
- Preparation and properties of glycols
- Oxidation by periodic acid and lead tetraacetate





#### Practice (4h)

- Functional group test for alcohol
- Distinction between primary and secondary alcohols with tertiary alcohols

#### Assignment (1h)

- Effect of substituents on Pinacol-Pinacolone rearrangement

### **Module-4: Phenols, ethers and epoxides**

#### Theory (4h)

- Preparation and properties, Acidity and factors affecting the acidic character of Phenol
- Ring substitution reactions, Reimer- Tiemann, Kolbe's-Schmidt Reactions, Fries and Claisen rearrangements with mechanism
- Preparation of Ethers and reactions with acids
- Preparation of Epoxides

#### Practice (4h)

- Functional group test for Phenol
- Separating components of a mixture by extraction using Ether

#### Assignment (1h)

- Reactions of epoxides with alcohol, ammonia derivatives, and  $\text{LiAlH}_4$ .

### **Module-5: Carbonyl Compounds-1**

#### Theory (4h)

- Structure, reactivity, and preparation of carbonyl compounds, Nucleophilic additions
- Nucleophilic addition-elimination reactions with ammonia derivatives with the mechanism
- Mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Claisen-Schmidt, Perkin, Cannizzaro reaction
- Wittig reaction, Beckmann and Benzil-Benzilic acid rearrangement

#### Practice (4h)

- Functional group test for Carbonyl compounds
- Silver mirror test for carbonyl compounds

#### Assignment (1h)

- Draw the mechanism of all the name reactions in this module

### **Module-6: Carbonyl Compounds-2**

#### Theory (4h)



- Haloform reaction and Baeyer Villiger oxidation, alfa- substitution reactions, oxidations and reductions (Clemmensen, Wolff-Kishner,  $\text{LiAlH}_4$ ,  $\text{NaBH}_4$ , MPV, PDC )
- Addition reactions of unsaturated carbonyl compounds: Michael addition, Active methylene compounds: Keto-enol tautomerism.
- Preparation and synthetic applications of diethyl malonate
- Preparation and synthetic applications of ethyl acetoacetate.

Practice (2h)

- Haloform test for carbonyl compounds

Assignment (1h)

- Reactivity order of Carbonyl compounds

### Module-7: Carboxylic Acids and their Derivatives and Sulfer containing compounds

Theory (6h)

- 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
- Preparation and reactions of thiols
- Preparation and reactions thioethers
- Preparation and reactions sulphonic acids

Practice (4h)

- Functional group test for carboxylic acid
- Hydrolysis of ester

Assignment (4h)

- Comparative study of nucleophilic substitution at acyl group -Mechanism of acidic and alkaline hydrolysis of esters
- Draw the mechanism of Claisen condensation, Dieckmann and Reformatsky reactions, Hofmann-bromamide degradation and Curtius rearrangement

*Reference Books:*

5.

### Course Outline

Code	Course Title	T-P-Pj (Credit)	Prerequisite
CUTM1475	Phase Equilibria and Chemical Kinetics	3-2-1	

### Objective

- The course gives idea about the different phases of matter and their equilibria from which the stability and sustainability can be easily predicted.
- Deals with kinetics study of different processes and surface phenomenon like adsorption, chemisorptions etc.

### Course outcomes

COs	Course outcomes	Mapping COs with POs (High-3, Medium-2, Low-1)
CO1	Knowledge on the fundamentals of different phases and kinetics of reaction.	PO1 (3)
CO2	Research and Problem Solving of kinetics based chemical reaction and degrees of freedom.	PO2 (3), PO4 (2)

### Course content

#### Module 1: Phase Equilibria-1 (8 hrs)

Definitions of phase, Concept of phases and Components; Degrees of freedom; Derivation of Gibbs Phase Rule for Non-reactive and reactive systems; Clausius-Clapeyron equation; Applications to solid-liquid, Liquid-vapour and Solid- vapour equilibria.

#### Module II: Phase Equilibria-2 (9 hrs)

Definition of phase diagram; Phase diagram for one component systems – water  
Phase diagram for one component systems – CO<sub>2</sub>, with applications; Liquid-vapour equilibrium for two component systems; Phase diagrams for systems of solid-liquid equilibria involving eutectic, congruent and incongruent melting points, solid solutions, Three component systems, water-chloroform-acetic acid system, triangular plots.

#### Practice 1

Determination of the solubility curve for phenol and water

### **Module III: Phase Equilibria-3 (8 hrs)**

Gibbs- Duhem-Margules equation and its derivation; 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.

#### **Practice 2**

Study the distribution law of Acetic acid and benzoic acid by water and carbon tetra chloride

### **Module IV: Chemical Kinetics-1 (12 hrs)**

Order and molecularity of a reaction; Rate laws in terms of the advancement of a reaction, rate constants; Differential and integrated form of rate expressions up to second order reactions; Pseudo first order reactions; Experimental methods of the determination of rate laws; Determination of order of a reaction by half-life and differential method; Kinetics of complex reactions (integrated rate Expressions up to first order only).

#### **Practice 3**

Kinetics Study on the Reaction between Sodium Thiosulphate and Hydrochloric Acid

#### **Practice 4**

Acid hydrolysis of methyl acetate with hydrochloric acid

### **Module V: Chemical Kinetics-2 (9 hrs)**

Opposing reactions and parallel reactions; Consecutive reactions and their differential rate equations (steady-state approximation in reaction mechanisms); Chain reactions; Temperature dependence of reaction rates; Arrhenius equation; activation energy; Unimolecular Reactions; Collision theory of reaction rates, Lindemann mechanism, qualitative treatment of the theory of absolute reaction rates.

#### **Practice 5**

Saponification value of ethyl acetate

#### **Practice 6**

Effect of ionic strength on rate of persulphate iodide reaction

### **Module VI: Catalysis (6 hrs)**

Types of catalyst, specificity and selectivity, mechanisms of catalyzed reactions at solid surfaces; Salt effects; effect of particle size and efficiency of nanoparticles as catalysts; Enzyme catalysis, Michaelis-Menten mechanism; Acid-base catalysis, turn-over number.

#### **Practice 7**

Study of the Catalytic Effects of Finely Divided Particles

### **Module VII: Surface Chemistry (12 hrs)**

Physical adsorption, chemisorptions; Freundlich and Langmuir adsorption isotherms; Multilayer adsorption and BET isotherm; Gibbs adsorption isotherm and surface excess, nature of adsorbed state.

#### **Practice 8**

Demonstration of the adsorption phenomena

#### **Practice 9**

Verify the Freundlich for adsorption of acetic acid on activated charcoal

#### **Practice 10**

Verify the Langmuir isotherm for adsorption of acetic acid on activated charcoal

#### *Text Books:*

1. Peter Atkins & Julio De Paula, Physical Chemistry 10th Ed., Oxford University Press (2014).
2. Castellan, G. W. Physical Chemistry, 4th Ed., Narosa (2004).
3. Levine, I. N. Physical Chemistry 6th Ed., Tata McGraw-Hill (2011).

#### *Reference Books:*

1. Engel, T. & Reid, P. *Physical Chemistry 3rd Ed.*, Prentice-Hall (2012).
2. Zumdhal, S.S. *Chemistry concepts and applications* Cengage India (2011).
3. Ball, D. W. *Physical Chemistry* Cengage India (2012).
4. Mortimer, R. G. *Physical Chemistry 3rd Ed.*, Elsevier: NOIDA, UP (2009).
5. Metz, C. R *Physical Chemistry 2nd Ed.*, Tata McGraw-Hill (2009).

### Course Outline

Code	Course Title	T-P-Pj (Credit)	Prerequisite
CUTM1476	Coordination Chemistry	3-2-1	

#### Objective

- To Know the basic of coordination chemistry, bio-inorganic chemistry and aimed at advanced knowledge in the field of industrial chemistry
- To be able to describe the stability of metal complexes by the use of formation constants and to calculate thermodynamic parameters from them
- To able to know the bonding and structure of coordination compounds and their applications

#### Course outcome

COs	Course outcomes	Mapping COs with POs (High-3, Medium-2, Low-1)
CO1	Able to gain knowledge and understand the fundamentals coordination chemistry and its application towards biological system.	PO1 (3)
CO2	Research and Problem Solving on rare earth elements and interpret the data for publication	PO2 (3), PO4 (2)
CO3	Design and development coordination complex molecule used as drug for different diseases like Wilson disease, cancer etc.	PO3 (3)

## Course content

### **Module-I (7Hours)**

#### **Coordination Chemistry**

Werner's theory, Valence bond theory (inner and outer orbital complexes), Electro neutrality principle and back bonding.

#### **Practice**

- To Synthesis and Characterization of Metal Complexes with Schiff Base Ligands
- Estimation of nickel (II) using Dimethylglyoxime (DMG).

### **Module-II (11Hours)**

#### **Crystal Field Theory**

Crystal field theory, measurement of  $10 Dq$  ( $\Delta_o$ ), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of  $10 Dq$  ( $\Delta_o$ ,  $\Delta_t$ ). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry. Qualitative aspect of Ligand field and MO Theory.

#### **Assignment -1**

#### **Practice**

To determine the crystal field stabilization energy (CFSE) of metal complexes.(V LAB )

### **Module-III(8 Hours)**

#### **Nomenclature of Coordination Compounds**

IUPAC nomenclature of coordination compounds, isomerism in coordination compounds. Stereochemistry of complexes with 4 and 6 coordination numbers. Chelate effect of polynuclear complexes, Labile and inert complexes.

#### **Assignment-2**

#### **Practice**

- To Prepare of Ferrous ammonium salt and estimation of Nitrogen
- Preparation and Analysis of Potassium Trioxalatoferate (III) Trihydrate

### **Module-IV(11 Hours)**

#### **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 & Bsworth diagrams). Difference between the first, second and third transition series. Chemistry of Ti, V, Cr Mn, Fe and Co in various oxidation states (excluding their metallurgy)

### **Assignment-3**

### **Assignment-4**

### **Practice**

- To estimate the amount of barium in the whole of the given solution of barium chloride
- Estimation of Iron in Hematite ore solution

### **Module-V (9hours )**

#### **Lanthanoids and Actinoids:**

Electronic configuration, oxidation states, colour, Spectral and magnetic properties, lanthanide contraction, separation of lanthanides (ion-exchange method only), Actinides elements and properties

### **Assignment-5**

### **Practice**

- To separate cation and anion from a unknown mixture by ion exchange column method
- Paper chromatographic separation of Ni(II) and Cu(II)

### **Module-VI(11Hours)**

#### **Bio-inorganic Chemistry-1:**

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 Carboxy peptidase. 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.

### **Assignment-6**

### **Assignment-7**

### **Assignment-8**

### **Practice**





- Preparation of Lyophilic and Lyophobic Sols
- Determination of Iron from a supplied waste water sample by redox and spectroscopic method

### Module-VII(7Hours)

#### Bio-inorganic Chemistry-2:

Iron and its application in bio-systems, Hemoglobin, Storage and transfer of iron.

#### Assignment-9

#### Assignment-10

#### Practice

Compare graphically the O<sub>2</sub> affinity of hemoglobin and myoglobin .

#### Recommended Books:

1. Purcell, K.F & Kotz, J.C. Inorganic Chemistry B. Saunders Co, 1977.
2. Huheey, J.E., Inorganic Chemistry, Prentice Hall, 1993.
3. Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry Panima Publishing Company 1994.
4. Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry Wiley-VCH, 1999
5. Bassolo, F, and Pearson, R.C. Mechanisms of Inorganic Chemistry, John Wiley & Sons, NY, 1967.
6. Greenwood, N.N. & Earnshaw A. Chemistry of the Elements, Butterworth-Heinemann, 1997.

#### Recommended Books For Practice:

1. Mendham, J., A. I. Vogel's Quantitative Chemical Analysis 6th Ed., Pearson, 2009

## Course Outline

### Heterocyclic Chemistry

Code	Course Title	T-P-P	Prerequisite
CUTM1477	Heterocyclic Chemistry	3-2-1	

#### Course Objectives

- To introduce students to Nitrogen containing functional groups and their application in organic conversions and related mechanisms.



- Students are also expected to learn about structure, synthesis, reactivity of important heterocyclic compounds and polycyclic aromatic hydrocarbons.
- To familiarize students about different classes of N-based naturally occurring important alkaloid and terpenoid compounds, their structures, synthesis and reactivity.

### Course Outcomes

COs	Course outcomes	Mapping COs with POs (High-3, Medium-2, Low-1)
CO1	Able to gain Knowledge on Nitrogen containing functional groups and their application, structure, synthesis, reactivity of important heterocyclic compounds and polycyclic aromatic hydrocarbons and different classes of N-based naturally occurring important alkaloid and terpenoid compounds, their structures, synthesis and reactivity	PO1 ( 3)
CO2	Research and Problem Solving	PO2(3), PO5(2)
CO3	Design and Development of organic molecules and their reaction mechanism	PO3(3), PO5(2)

### Course Content

#### Module-I (5 Hrs.)

##### **Nitrogen Containing Functional Groups: Nitro compounds, nitriles and isonitriles**

Structure and Preparation of nitroalkanes and nitroarenes

Properties and reactions of nitroalkanes

Properties and reactions of nitroarenes

Structure, Preparation and properties of nitriles and isonitriles

Assignment 1/Flip class: Important Nitro aromatic compounds and their uses

#### Module-II (8 Hrs.)

##### **Nitrogen Containing Functional Groups: Amines**

Preparation of primary amines: Reduction of nitro compounds, Hofmann ammonolysis, Hofmann degradation, Gabriel phthalimide synthesis.

Preparation of secondary and tertiary amines: Aminolysis of alkyl halides, Reductive amination of aldehydes and ketones, Ullmann reaction

Properties of amines, Basicity, Effect of substituent and solvent on basicity.

Important reactions of amines: Alkylation, acylation, Carbylamine reaction

Important reactions of amines: Mannich reaction, Hoffmann's exhaustive methylation, Hofmann-elimination reaction

Diazonium Salts: Structure, Preparation and reactions/applications

Assignment 2/Flip class: Electrophilic substitution reactions of aryl amines

Assignment 3/Flip class: Distinction between 1°, 2° and 3° amines with Heinsberg reagent and nitrous acid.

### **Laboratory Practices (Module I and II): (13.30 hrs.)**

1. Detection of extra elements (Nitrogen)
2. Detection of extra elements (Sulphur)
3. Detection of extra elements (Halogens)
4. Functional group test for: Nitro groups
5. Functional group test for: Amine groups
6. Functional group test for: Amide groups

Module-III (8 Hrs.)

#### **Five membered Heterocyclic Compounds containing one heteroatom:**

Classification, nomenclature and structure of pyrrole, furan and thiophene (5-numbered) and pyridine (6-membered)

Molecular orbital pictures and aromaticity in of pyrrole, furan and thiophene and pyridine

Synthesis, reactions and mechanism of substitution reactions of: Furan

Synthesis of Pyrrole: Knorr pyrrole synthesis, Paal-Knorr synthesis, Hantzsch synthesis.

Reactions and mechanism of substitution reactions of Pyrrole

Derivatives of furan: Furfural and furoic acid.

Assignment 4/Flip class: Synthesis and Properties of thiophene

Assignment 5/Flip class: Acidic and basic character of Pyrrole, Furan and Thiophene

Module-IV (6 Hrs.)

#### **Six membered and condensed Heterocyclic Compounds:**

Structure, synthesis and properties of Pyridine (Hantzsch synthesis), Pyrimidine

Structure elucidation of indole, Fischer indole synthesis and Madelung synthesis)

Structure elucidation of quinoline and isoquinoline

Skraup synthesis, Friedlander's synthesis

Assignment 6/Flip class: Knorr quinoline synthesis, Doebner- Miller synthesis

Assignment 7/Flip class: Bischler-Napieralski reaction, Pictet-Spengler reaction, Pomeranz-Fritsch Reaction.

### **Module-V (5 Hrs.)**

#### **Polynuclear Hydrocarbons:**

Preparation and structure elucidation of naphthalene

Reactions of naphthalene

Important derivatives of naphthalene

Preparation, structure elucidation and important derivatives of anthracene.

Assignment 8/Flip class: Preparation, structure elucidation and properties of phenanthrene

### **Module-VI (6 Hrs.)**

#### **Alkaloids**

Natural occurrence, Isolation and their physiological action

General structural features, experimental determination

Hoffmann's exhaustive methylation, Emde's modification.

Structure elucidation and synthesis of Hygrine

Structure elucidation and synthesis of Nicotine.

Assignment 9/Flip class; Medicinal importance of Nicotine, Hygrine, Quinine, Morphine, Cocaine, and Reserpine

Laboratory Practices: (11.30 Hrs.)

7. Qualitative analysis of unknown organic compounds containing simple functional groups: Alcohol

8. Qualitative analysis of unknown organic compounds containing simple functional groups: Carboxylic acids

9. Qualitative analysis of unknown organic compounds containing simple functional groups: Phenols

10. Qualitative analysis of unknown organic compounds containing simple functional groups: Carbonyl compounds (aldehyde)

11. Qualitative analysis of unknown organic compounds containing simple functional groups: (ketones)

### **Module-VII (3 Hrs.)**

#### **Terpenoids:**

Occurrence, classification, isoprene rule;

Elucidation of structure and synthesis of Citral, Neral

Assignment 10/Flip class: Elucidation of structure and synthesis of  $\alpha$ -terpineol.

**Text Books :**

1. A Textbook of Organic Chemistry – III, M. K. Jain, S. C. Sharma, Amita, Vishal Publishing Co.
2. Kalsi, P. S. Textbook of Organic Chemistry 1st Ed., New Age International (P) Ltd. Pub.
3. Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education)
4. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Organic Chemistry, Oxford University Press.

**Reference Books :**

1. Acheson, R.M. Introduction to the Chemistry of Heterocyclic compounds, John Welly & Sons (1976).
2. Heterocyclic Chemistry, Fifth Edition, J. A. Joule, K. Mills and G. F. Smith
3. Singh, J.; Ali, S.M. & Singh, J. Natural Product Chemistry, PragatiParakashan (2010).

**Course Outline**

Code	Course Title	T-P-P (Credit)	Prerequisite
CUTM1478	Electrochemistry	3-2-1	

**Objective**

- To Know the basic of ions, electrolyte, movement of ions, electrochemistry
- To know how the ionic movements are related to different other fields such as thermodynamics.
- Also, this course will help students to garner basic knowledge on novel energy storage devices

**Course outcome**

COs	Course outcomes	Mapping COs with POs (High-3, Medium-2, Low-1)
CO1	Able to gain Knowledge on basic of ions, electrolyte, movement of ions, electrochemistry, behavior of ions in	PO1 ( 3)

	solution phase under different conditions and its application towards different energy storage devices	
CO2	Research and Problem Solving	PO2(3), PO5(2)
CO3	Design and Development of electrolytes and electrochemical devices.	PO3(3), PO5(2)
CO5	Analytical and Computational Skill	PO5(3)

### Course content

#### **Module-I: Conductance I(12 hrs)**

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.

**Practice 1:** Electrolyte solution

**Practice 2:** Electrolytic conductance

**Assignment 1:** Molar conductivity and their variation with dilution for weak and strong electrolytes.

**Assignment 2:** Ostwald's dilution law.

#### **Module-II: Conductance II(5hrs)**

Walden's rules, Debye-Huckel-Onsager equation. Ionic mobility and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary methods.

**Assignment 3:** Walden's rules, Debye-Huckel-Onsager equation

**Assignment 4:** Ionic mobility and their determinations, transference numbers and their relation to ionic mobilities.

#### **Module-III: Conductance III (6 hrs)**

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.

**Practice 3:** Conductometric titrations

**Assignment 5:** Applications of conductance measurement for determining hydrolysis constants of salts.

#### **Module-IV: Electrochemistry I(17 hrs)**

Quantitative aspects of Faraday's laws of electrolysis, applications of electrolysis in metallurgy and industry. Electrochemical series, rules of oxidation/reduction of ions based on half-cell potentials. Nernst equation; Standard electrode (reduction) potential and its application to different kinds of half-cells. Electromotive force of a cell and its measurement. Chemical cells, reversible and irreversible cells with examples.

**Practice 4:** Application of electrolysis in Electroplating

**Practice 5:** Electrochemical series application

**Practice 6:** Electrochemical cell

**Practice 7:** Nernst equation

**Practice 8:** Cell potential determination

**Assignment 6:** Quantitative aspects of Faraday's laws of electrolysis

**Assignment 7:** Applications of electrolysis in metallurgy and industry.

#### **Module-V: Electrochemistry II(8 hrs)**

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, and glass 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).

**Assignment 8:** Concentration cells without transference.

### **Module-VI: Electrical & Magnetic Properties of Atoms and Molecules(6 Hrs)**

Basic ideas of electrostatics, dielectric constant, Dipole moment and molecular polarizabilities and their measurements. Basics of diamagnetism, paramagnetism. Magnetic susceptibility and its measurement.

**Practice 9:** Static electricity

**Assignment 9:** Basic ideas of electrostatics, dielectric constant.

### **Module-VII: Energy Storage and Conversion(12 Hrs.)**

Fundamentals on Li ion batteries, basic principle and types of fuel cells, theory of solar cells and types of solar cells, basic principles on super capacitors and types of super capacitors.

**Practice 10:** Solar Panel Experiment

**Practice 11:** Photoelectric effect

**Practice 12:** Super capacitor preparation

**Assignment 10:** Needs for energy storage and storage alternatives.

#### *Text Books:*

1. Atkins, P.W & Paula, J.D. Physical Chemistry, 10th Ed., Oxford University Press (2014).
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).

### **Course Outline**

Code	Course Title	T-P-Pj (Credit)	Prerequisite
CUTM1479	Biomolecules	3-2-1	

#### **Objective**

- To Know the basic of Bio-Organic chemistry and its application in industry





- This course gives idea about the structure of different bases of nucleic acid, DNA and RNA.
- Number of amino acids, their functions and the peptide bond that connect di, tri and polypeptides.
- To study about proteins, lipid and carbohydrates

### Course outcomes

COs	Course outcomes	Mapping COs with POs (High-3, Medium-2, Low-1)
CO1	Able to gain Knowledge on Bio-Organic chemistry and its application in industry, structure of different bases of nucleic acid, DNA and RNA, Number of amino acids, their functions and the peptide bond that connect di, tri and polypeptides, proteins, lipid and carbohydrates	PO1 (3), PO9(1)
CO2	Research and Problem Solving for various diseases	PO2(3), PO5(2)
CO3	Design and Development of Diagnostic kit and Device fabrication	PO3(3), PO5(2)
CO5	Analytical and Computational Skill	PO5(3)

### Course content

#### **Module I: Nucleic Acids (8 h)**

Nucleic Acids: Introduction of Nucleic Acids, Components of nucleic acids, Nucleosides and

nucleotides, Structure, synthesis and reactions of: Adenine, Guanine, Cytosine, Uracil and Thymine, Structure of polynucleotides.

**Practice 1:** Isolation and characterization of DNA from cauliflower

**Practice 2:** Isolation and characterization of DNA from onion

**Assignment 1:** Structure of polynucleotides

### **Module II: Amino acids, peptide and proteins (13 h)**

Amino acids, peptide and proteins: Introduction to amino acid, peptide and protein, Classification of amino acid and peptides,  $\alpha$ -Amino Acids: Synthesis, ionic properties and reactions, Zwitterions, pKa 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)

**Practice 3:** Estimation of glycine by Sorenson's formalin method

**Practice 4:** Study of the titration curve of Amino acid

**Practice 5:** Estimation of proteins by Lowry's method.

**Assignment 2:** Reactions, Zwitterions, pKa values, isoelectric point and electrophoresis

**Assignment 3:**  $\alpha$ -Amino Acids: Study of peptides: determination of their primary structures-end group analysis

### **Module III: Enzymes (6 h)**

Enzymes: Introduction, classification and characteristics of enzymes, Salient features of active site of enzymes, Mechanism of enzyme action, Factors affecting enzyme action, Coenzymes and Cofactors and their role in biological reactions, specificity of enzyme action (including stereospecificity), Enzyme inhibitors: Importance of enzyme inhibition phenomenon of inhibition (competitive, uncompetitive and non-competitive inhibition including allosteric inhibition).

**Assignment 4:** Enzyme inhibitors: Importance of enzyme inhibition phenomenon of inhibition (non-competitive inhibition including allosteric inhibition)

### **Module IV: Lipids (10 h)**

Lipids: Introduction to oils and fats (Properties and functions), Classes of Lipids (common fatty acids present in oils and fats, Examples of diff. Lipids), Hydrogenation of fats and oils, Saponification value, acid value, iodine number, Reversion and rancidity

**Practice 6:** Saponification value of an oil or a fat

**practice 7:** Determination of Iodine number of an oil/ fat.

**Module V: Concept of Energy in Biosystems (8 h)**

Concept of Energy in Biosystems: Introduction to metabolism (catabolism, anabolism), ATP: ATP hydrolysis and free energy change, Biological redox systems: NAD<sup>+</sup>, FAD, Conversion of food to energy, Outline of catabolic pathways of carbohydrate- glycolysis, Fermentation and Krebs cycle, Catabolic pathways of fat and protein, Metabolic pathways of protein, fat and carbohydrate

**Practice 8:** Extraction of starch from potatoes

**Assignment 5:** Outline of catabolic pathways of carbohydrate-glycolysis, Fermentation and Krebs cycle

**Assignment 6:** Catabolic pathways of fat and protein, Metabolic pathways of protein, fat and carbohydrate

**Module VI: Pharmaceutical Compounds (9 h)**

Pharmaceutical Compounds: Structure and Importance: Classification, structure and therapeutic uses of antipyretics: Paracetamol (with synthesis), Analgesics: Ibuprofen (with synthesis), Antimalarials: Chloroquine, Antibiotics and detailed study of chloramphenicol, Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine)

**Practice 9:** Preparation of triphenylmethanol via Grignard

**Practice 10:** Handling Pyrophoric Materials like n-Butyl Lithium

**Assignment 7:** Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine)

**Module VII (12 h)**

Bio-imaging and Bio-Medical science: Introduction to basic cell biology, Optical fluorescent probe and photophysical property, Optical probe for bio-imaging application, Protein labelling, Diagnostic kit and Device fabrication

**Practice 11:** Live Cell Imaging using small molecular probe

**Practice 12:** Fluorescent Labelling of COS-7 Expressing SNAP-tag Fusion Proteins for Live Cell Imaging

**Assignment 8:** Diagnostic kit development

## Assignment 9: Device fabrication

### Reference 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.

## Course Outline

### Nomenclature

Code	Course Title	T-P-P (Credit)	Prerequisite
CUTM1480	Quantum Chemistry and Spectroscopy	3-2-1	

### Objective

<ul style="list-style-type: none"> <li>• To impart knowledge about quantum mechanical principles and understanding as well as predicting different microscopic phenomena.</li> <li>• To understand the covalent nature of bonding and their theoretical background and correlation to practical aspects.</li> <li>• To have a sound understanding of different spectroscopic techniques and photochemistry.</li> </ul>
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### Course outcome

COs	Course outcomes	Mapping COs with POs (High-3, Medium-2, Low-1)
CO1	Able to gain Knowledge on quantum mechanical principles and understanding as well as predicting different microscopic phenomena, concepts of covalent bonding between atoms, their stability, which has important industrial applications and different spectroscopic techniques and photochemistry	PO1 ( 3),PO9(1)

CO2	Research and Problem Solving in pharmaceutical as well as quantum and classical field of Chemistry	PO2(3), PO5(2)
CO3	Design and Development of structural aspects of compounds which has huge application in pharmaceutical as well as different research fields	PO3(3), PO5(2)
CO5	Analytical and Computational Skill by using various softwares for quantum computing.	PO5(3)

### Course content

#### **Module I Quantum Chemistry (18 hours)**

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, Heisenberg Uncertainty principle; wavefunctions, probability distribution functions, nodal properties, 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.

#### **Assignment 1**

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).

#### **Assignment 2**

##### **Practice:**

Eigen systems: Geometrical Interpretation (**v-lab**)

Geometry Optimization using ab-initio quantum calculations (**v-lab**)

## Module II

### Chemical bonding (5 hours)

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.

### Assignment 3

## Module III (3 hours)

### Introduction to 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.

### Assignment 4

## Module IV

### Vibrational spectroscopy (7 hours)

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.

### Assignment 5

### Practice

- Calculation of Vibrational Frequency of Molecules and Visualization of Normal Modes
- Instrumentation and working principles of solutions infra red (IR) spectroscopy (**v-lab**)

## Module V

### Raman and Electronic Spectroscopy (10 hours)

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.

#### Assignment 6

#### Assignment 7

#### Practice

- Study the 200-500 nm absorbance spectra of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  (in 0.1 M  $\text{H}_2\text{SO}_4$ ) and determine the  $\lambda_{\text{max}}$  values. Calculate the energies of the two transitions in different units ( $\text{J mol}^{-1}$ ,  $\text{kJ mol}^{-1}$ ,  $\text{cm}^{-1}$ , eV).
- Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of  $\text{K}_2\text{Cr}_2\text{O}_7$ .
- 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.

## Module VI (6 hours)

**Nuclear Magnetic Resonance (NMR) spectroscopy:** Principles of NMR spectroscopy, Larmor precession, chemical shift and low resolution spectra, different scales, spin-spin coupling and high resolution spectra, interpretation of PMR spectra of organic molecules.  
**Electron Spin Resonance (ESR) spectroscopy:** Its principle, hyperfine structure, ESR of simple radicals.

#### Assignment 8

#### Practice

Nuclear magnetic resonance spectroscopy and evaluation of simple  $^1\text{H}$  NMR spectra of select organic compounds (**v-lab**)

## Module VII Photochemistry (16 hours)

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.

#### Assignment 9

## Assignment 10

### Practice:

- **Spectrophotometry (v-lab)**
- 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
- Determine the amount of iron present in a sample using 1,10-phenanthroline.
- Determine the dissociation constant of an indicator (phenolphthalein).
- Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.

### Reference Books:

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

**Practice 1.** 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

**Practice 2.** Determine the concentrations of  $\text{KMnO}_4$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  in a mixture.

**Practice 3.** Study the kinetics of iodination of propanone in acidic medium.

**Practice 4.** Determine the amount of iron present in a sample using 1,10-phenanthroline.

**Practice 5.** Determine the dissociation constant of an indicator (phenolphthalein).

**Practice 6.** Study the kinetics of interaction of crystal violet/ phenolphthalein with sodium hydroxide.

### Reference Books

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





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

### Course Outline

Code	Course Title	T-P-Pj (Credit)	Prerequisite
CUTM1481	<b>Organometallic Chemistry</b>	<b>3-2-1</b>	

### Objective

- The main focus of this course is on the synthesis, structure, bonding, properties and reactivity of organometallic compounds such as: metal carbonyls, hydrocarbon, and carbocyclic based molecules.
- This course also covers, 18-electron rule (Saturation and Unsaturation), Organometallic reaction (substitution, oxidative-addition, reductive elimination, insertion and de-insertion, and isomerization).

### Course outcome

COs	Course outcomes	Mapping COs with POs (High-3, Medium-2, Low-1)
CO1	Able to gain Knowledge on synthesis, structure, bonding, properties and reactivity of organometallic compounds such as: metal carbonyls, hydrocarbon, and carbocyclic based molecules, 18-electron rule (Saturation and Unsaturation), Organometallic reaction (substitution, oxidative-addition, reductive elimination, insertion and de-insertion, and isomerization).	PO1 ( 3),PO9(1)

CO2	Research and Problem Solving by using modern methods to characterize organo metallic compounds	PO2(3), PO5(2)
CO3	Design and Development of mechanisms and how to combine these to understand efficient catalytic processes	PO3(3), PO5(2)
CO5	Analytical and Computational Skill	PO5(3)

### Course content

#### **Module-I (8hours)**

Organometallic Compounds Definition and classification of organometallic compounds, The different organometallic Compounds the basis of bond type. Concept of hapticity of organic ligands.

**Assignment -1/Flip-class-1 :** Concept of hapticity of organic ligands

**Practice -1 :** Estimation of Fe(II) with  $K_2Cr_2O_7$

**Practice -2:** Estimation of Copper in the alloyed brass

#### **Module-II (12hours)**

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. Organometallic Compounds with metal-metal bond Cluster. Structures of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni using VBT. Pi-acceptor behaviour of CO (MO diagram of CO to be discussed).

**Assignment -2/Flip-class-2 :** Pi-acceptor behaviour of CO (MO diagram of CO to be discussed)

**Practice -3 :** To detect the presence of a cation and anion in a given inorganic mixture.

**Practice -4:** Identifying Ions

#### **Module-III (9hours)**

Synergic effect organometallic compounds having ligands with back bonding as metal carbonyl, metal carbenes, metal nitrosyls, IR data to explain extent of back bonding.

**Assignment -3/Flip-class-3** : IR data to explain extent of back bonding

**Practice -5** :Qualitative analysis of cations part

**Practice -6**:Test for cobalt ions cation analysis, Identification of Nickel ions in chemistry Lab

**Module-IV(11hours)**

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 trialkylaluminium (dimer), concept of multicentre bonding in these compounds. Role of triethylaluminium in polymerisation of ethene (Ziegler - Natta Catalyst). Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Structure and aromaticity.Comparison of aromaticity and reactivity with that of benzene.

**Assignment -4/Flip-class-4** : Concept of multicentre bonding in these compounds.

**Assignment -5/Flip-class-5**: Structure and aromaticity.Comparison of aromaticity and reactivity with that of benzene.

**Assignment -6/Flip-class-6** : Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation).

**Practice -7** : Cations (Zn(II), Al(III), Cu(II), Fe(II) and Fe(III): Tested with NaOH

**Practice -8**: Bromide ion test by organic layer test in chemistry lab,  
Brown ring test for nitrate ion in laboratory.

**Practice -9** : Silver nanoparticles synthesis from plant extract

**Practice -10**: Synthesis of Copper Sulphate ( $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ )

**Module**

**V(5hours)**

Reaction Kinetics and Mechanism 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.

**Module VI (6 hours)**

Thermodynamic and Kinetic stability, Kinetics of octahedral substitution, Ligand field effects and reaction rates, Mechanism of substitution in octahedral complexes. Catalysis by Organometallic Compounds

**Assignment -7/Flip-class-7** : Mechanism of substitution in octahedral complexes.Catalysis by Organometallic Compounds

**Assignment -8/Flip-class-8** : Kinetics of octahedral substitution ,Ligand field effects and reaction rates

**Practice -1 1:** Estimation of free alkali present in different soaps/detergents

**Module-VII(8hours)**

Study of the following industrial processes and their mechanism: 1. Alkene hydrogenation (Wilkinsons Catalyst),Hydroformylation (Co salts),Wacker Process,Synthetic gasoline (Fischer Tropsch reaction).

**Assignment -9/Flip-class-9:** Study of the following industrial processes and their mechanism: 1. Alkene hydrogenation (Wilkinsons Catalyst),Hydroformylation (Co salts)

**Assignment -10/Flip-class-10:** Synthetic gasoline (Fischer Tropsch reaction) ,Wacker Process.

**Practice -1 2:** Estimation of Fe(II) and oxalic acid using standardized  $\text{KMnO}_4$  solution.

**Text Books:**

1. Inorganic Chemistry ; Ajay kumar
- 2.Inorganic Chemistry By Madan Malik Tuli
- 3.principal of inorganic chemistry by puri sharma kalia

**Reference Books:**

1. Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson,2006.
2. Sharpe, A.G. Inorganic Chemistry, 4th Indian Reprint (Pearson Education) 2005
3. Douglas, B. E.; McDaniel, D.H. & Alexander, J.J. Concepts and Models in Inorganic Chemistry 3rd Ed., John Wiley and Sons, NY, 1994.
4. Greenwood, N.N. & Earnshaw, A. Chemistry of the Elements, Elsevier 2nd Ed, 1997 (Ziegler Natta Catalyst and Equilibria in Grignard Solution).
5. Lee, J.D. Concise Inorganic Chemistry 5th Ed., John Wiley and sons 2008.
6. Powell, P. Principles of Organometallic Chemistry, Chapman and Hall, 1988

**Course outline**

**Nomenclature**

Code	Course Title	T-P-Pj (Credit)	Prerequisite
CUTM1482	Spectroscopy	3-2-1	

## 1. Objective

- To learn proper sample handling procedures for acquiring infrared **spectra**.
- To determine the percentage composition of a liquid sample mixture by the application of Beer's law.
- Recognize and draw particular carbohydrate structures
- Know general structural elements of cyclic monosaccharides and disaccharides, and their implications for structure/function
- To train the students for identification of unknown compounds
- To train the students to synthesise various dyes

## 2. Learning outcome

- Explain what it means to use spectroscopic methods for qualitative and quantitative analysis.
- Identify the terms in and describe deviations to Beer's Law.
- Describe the effect of changing the slit width and the impact it will have on qualitative and quantitative analyses
- Describe/recognize amino acid structures, describe their physical and chemical properties, and predict how their ionic charges change with pH.
- Define primary, secondary, tertiary and quaternary structure in proteins and identify the types of interactions important in each case.
- Describe the chemical nature of enzymes and their function in biochemical reactions.
- Explain what happens during digestion of proteins, catabolism of amino acids and the urea cycle.
- Can predict proton nmr of organic compounds
- Can perform chromatographic techniques for separation of mixture of compounds
- Able to identify the structure of an unknown organic compound
- Can synthesise various dyes

COs	Course outcomes	Mapping COs with POs (High-3, Medium-2, Low-1)
CO1	To impart knowledge of basic concepts of spectroscopy	PO1 ( 3), PO2 (2), PO4(1)
CO2	Understanding of the problem solving techniques of organic spectroscopy	PO1 ( 2),PO2(3), PO5(2)
CO4	Investigation of different patterns of peaks and their origin and hence deduction of structure of organic species.	PO2(2), PO4(2), PO5(3)
CO5	To develop analytical skills on predicting and explaining the various spectroscopic patterns for organic molecules	PO2(3), PO4(3), PO5(2)

### Course Content

#### **Module -1(UV-VIS Spectroscopy)**

**6 hrs**

Introduction to UV spectroscopy, Theory and principles, Types of electronic transitions, T<sub>max</sub>, Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; of Application Woodward rules for calculation of  $\lambda_{max}$  for the following systems:  $\alpha,\beta$  unsaturated aldehydes, ketones, carboxylic acids and esters; Conjugated dienes: distinction between cis and trans isomers.

**Assignment-1:**Types of electronic transitions, T<sub>max</sub>, Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption

**Practice-1:** To study the UV-Visible Spectroscopy of Conjugated Molecules

**Practice-2:** Solvent Effects on the UV-visible Absorption Spectra

**Practice-3:** To Determine of the Molar Absorptivity of a Light Absorbing Molecule by using Lambert-Beer's law

#### **Module-2 (IR Spectroscopy)**

**6hrs**

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

**Assignment-2:**IR absorption positions of O, N and S containing functional groups

**Assignment-3:** Fingerprint region and its significance

**Practice-4:** To Calculate Vibrational Frequency of Molecules and Visualization of Normal Modes

### **Module -3 (NMR Spectroscopy)**

**6 hrs**

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

**Assignment-4:** chemical shift and factors influencing it

**Assignment-5:** Spin - Spin coupling and coupling constant

**Practice-5:** Nuclear magnetic resonance spectroscopy and evaluation of simple  $^1\text{H}$  NMR spectra of select organic compounds

**Practice-6:** Identification of unknown components using spectroscopic techniques

### **Module-4(Mass spectroscopy)**

**5 hrs**

Introduction to mass spectrometry, Ionization methods & mass filter techniques in mass spectrometry, ionization methods(electron impact, chemical ionization), molecule fragmentation, Mac-Lafferty rearrangement

**Assignment-6:** Mac-Lafferty rearrangement

**Practice-7:** Instrumentation and working principles principles of mass spectroscopy

### **Module-5(Carbohydrates)**

**7 hrs**

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: starch, cellulose and glycogen.

**Assignment-7:** epimers and anomers

**Assignment-8:** mutarotation

**Practice-8:** To estimate the blood glucose level by glucose oxidase method

**Practice-9:** Action of Salivary Amylase on Starch

### **Module – 6 (Dyes)**

**6hrs**

Classification, Colour and constitution; Mordant and Vat Dyes; Chemistry of dyeing; 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.

**Assignment-9:** Mordant and Vat Dyes



**Practice-10:** synthesis of fluorescein dye from marker ink and phthalic anhydride

**Practice-11:** Methyl Orange: Organic synthesis

Module-7 (**Chromatography**)

**4hrs**

Gas Chromatography, Column Chromatography, supercritical fluids, TLC, HPLC

**Assignment-10:** TLC and supercritical fluids

**Practice-12:** Separation of compounds using column chromatography

### 3. Reference

#### *Text Books:*

1. Organic spectroscopy by Y.R Sharma
2. Instrumental Methods of Chemical Analysis by B.K Sharma
3. Singh, J.; Ali, S.M. & Singh, J. Natural Product Chemistry, Prajati Prakashan (2010).
4. Kalsi, P. S. Textbook of Organic Chemistry 1st Ed., New Age International (P)Ltd. Pub.

#### *Reference Books:*

1. Organic spectroscopy by William Kemp
2. Morrison, R. T. & Boyd, R. N. Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education)
3. Spectrophotometric identification of Organic Compounds by Silverstein
4. Billmeyer, F. W. Textbook of Polymer Science, John Wiley & Sons, Inc. 4. Gowariker, V. R.; Viswanathan, N. V. & Sreedhar, J. Polymer Science, New Age International (P) Ltd. Pub.
5. Finar, I. L. Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
6. Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Organic Chemistry, Oxford University Press.
7. Pavia, D. L. et al. Introduction to Spectroscopy 5th Ed. Cengage Learning India Ed. (2015).

## Renewable Energy Applications

Learning Outcomes:



Upon successful completion of this subject, students should be able to

1. Know in depth of materials of Sustainable energy products and it's applications.
2. Explain basics of Renewable energy technologies and it's applications.
3. Increased awareness about solar thermal technology.
4. Become industry-ready in Entrepreneurship.

### **Material for Renewable Energy application**

#### Module -1

Basic fundamentals of different types semiconductors (Energy band, charge carriers and their motion, generation, recombination, doping)

**Practice:** Crystal structure, phase identification and crystallite size determination of PV materials by XRD (using Biovia MS and phase identification by using relevant software)

Photovoltaic Cell - Construction & Working (Si based)

Practice: UV visible analysis of photovoltaic material

Concept of various types PN junction .

Practice: Measurement of photo luminescence (PL) behavior of photovoltaic material

Role of materials for sustainable development of next generation photovoltaic cells

Practice: To study crystallites (grain) size and strain through *Williamson-Hall plot* method

Efficiency calculation of solar cell

Practice: To determine the resistivity of semiconductors by Four probe Method.

Nano-Photovoltaic (Graphene/CNT, ZNO, TiO<sub>2</sub>)

Practice: Study of Hall effect (Determination of nature of charge carriers in a semiconductor)

Composite materials for solar cell (Graphene/Al, TiO<sub>2</sub>-SiO<sub>2</sub> composite for solar cell)

Perovskite based solar cell (transition metal doped PbTiO<sub>2</sub>)

Dye-sensitized solar cells

Materials (Al/hybrid glass-carbon fiber) for wind energy conversion

Text Book:

1. Vincent, D. , Materials for Sustainable Energy, Nature publishing group, 2010.
2. Paranthaman, M. Parans, Wong-Ng, Winnie, Bhattacharya, Raghu N (Eds.), Semiconductor Materials for Solar Photovoltaic Cells, Springer, 2015.

Reference Book:

1. Sabu, T., El HadjiMamour, S., Nandakumar, K., Samuel, O., Jihuai, W., Nanomaterials for Solar Cell Applications, Elsevier, 2019.
2. Peter, P. Rogers, Kazi F. Jalal, John A. Boyd, An introduction to sustainable development, Glen Educational Foundation, 2008.

**2. Renewable Energy Technology for Industrial Process (48 hrs)**

Relevance of economic and financial viability evaluation of renewable energy technologies,

Renewable Energy Policies of India and in the state of Odisha

Practice: Site visit for acquire knowledge on different renewable energy technologies and it's system

Basics of light to energy conversion and Concept on solar PV

Practice: Measurements and estimation of solar radiation

Concept of mono-crystalline, poly-crystalline, amorphous

Practice: Identify and specify different types of components used in a solar PV system

New generation of Solar cell, working principle and applications

Practice: Simulation of solar cell by using PVSOL software

Effects of parameters on PV module power and efficiency

Practice: VI characteristics of solar cell/module

Concept on Concentrated solar thermal (CST)

Practice: Temperature tracking of solar cell/module

Concentrated solar power (CSP), new technology of solar thermal

Practice: Performance of Solar PV module at varying tilt angle

Concept of wind energy, Basic laws and efficiency limit for wind energy conversion

Practice : Modeling of solar cooker

Concept of aerodynamics effects

Practice : Modeling of solar flat plate collector

description of horizontal and vertical axis wind turbine

Practice: Generation of electricity by wind machines

Concept on Biomass, Electricity generation from biomass.

Practice: Maximum power point tracking of a wind turbine

Practice: Performance testing of bio diesel in VCR machine

Text Books:

1. D. P. Kothari, K. C. Singal and R. Ranjan, Renewable Energy Sources and Emerging Technologies, Second Edition, PHI Learning Pvt. Ltd, New Delhi, 2011.
2. C. S. Solanki, Photovoltaic – Fundamentals, Technologies and Applications, PHI Learning Pvt. Ltd., 2011.

Reference Book:

1. V. V. N. Kishore, Renewable Energy Engineering and Technology: principles and practice, Teri, India, 2008.
2. Hakeem, Khalid Rehman, Jawaid, Mohammad, Rashid, Umer (Eds.), Biomass and Bioenergy Applications, Springer, 2014.
3. S. S. Das, D. D. Behera, and A. Pradhan, Clean Energy Products: A Path for Attaining Livelihood Security, Notion Press, and ISBN: 9781636691602, 2020.
4. S. S. Das, D. D. Behera, and N. C. Giri, Clean Energy Applications in Modern World, Notion Press, ISBN: 9781638069560, 2021.

### **Micro-grid Design and Implementation (36 hrs)**

Practice: Site survey (1 kW or 1MW)

Practice: Sizing of micro grid system (1kW/1MW)

Practice: Single line diagram of micro grid system

Practice: Identify and specify different components used in a micro grid system

Practice: Connection practice of solar modules in a micro grid system

Practice: Designing of micro grid system

Practice: Analysis of micro grid system

Practice: Designing of micro grid system with battery storage

Practice: Performance calculation of micro grid system

Practice: Connection practice of CCR/Inverter in a micro grid system

Practice: Test, record and verify the power quality of a micro grid system

Practice: O & M of micro grid system

Text Books:

1. Suneal Deambi, Photovoltaic System Design: Procedures, Tools and Applications, CRC Press, 2018.
2. Miguel Castilla, Antonio Carlos Zambroni de Souza, Microgrids Design and Implementation, Springer, 2019.

Reference Books:

1. S. S. Das, D. D. Behera, and N. C. Giri, Clean Energy Applications in Modern World, Notion Press, ISBN: 9781638069560, 2021.
2. Federico Delfino, Renato Procopio, Massimo Brignone, Michela Robba, Mansueto Rossi, Stefano Bracco, Microgrid Design and Operation: Toward Smart Energy in Cities, Artech House, London, 2018

#### **4. Hybrid Renewable Energy System (48 hrs)**

Global scenario of Hybrid renewable energy system, integrated renewable energy systems with input sources

Practice: Modeling of renewable energy systems integrated renewable energy systems with input sources

Practice: Connection practice of Solar PV-T System

Selection of technology and components for hybrid renewable systems.

Practice: Designing of solar PV system (On-grid/Off-grid)

Concept of hybrid solar PVT system

Practice: Designing of hybrid solar-thermal system

Selection of Components for Hybrid solar PV-T system

Practice: Analysis of hybrid solar-thermal system

Synchronization process of renewable systems.

Practice: Connection practice of PV-wind system

Operation of hybrid PV and wind system

Practice: Modeling of wind power system

Concept of hybrid PV and wind system and its components

Practice: Demonstration of Load curve in the plant

Load curve

Practice: Study the dynamic behavior of wind turbines

Concept of Hybrid PV and hydro system and its components

Practice: Modeling of hydro power system

Concept of hybrid PV and Biomass system and its components

Practice: Chemical composition of biomass system

. Practice: Emission testing of bio diesel/bio ethanol in gas analyzer

Text Books:

1. S. Sukhatme and J. Nayak: Solar Energy: Principle of Thermal collection and storage, Third Edition ( Tata McGraw-Hill, 2008)
2. C. S. Solanki: Solar Photovoltaic – Fundamentals, Technologies and Applications, PHI.

Reference Books:

1. Ersan Kabalci, Hybrid Renewable Energy Systems and Microgrids,
2. V. N. Kishore, Renewable Energy Engineering and Technology: principles and practice, Teri, India, 2008.
3. N. C. Giri, S. R. Nayak, S. P. Mishra, and S. N. Sahu, Project Management and Smart Electrical Systems, ISBN 9798587652200, Amazon; 1st edition, 27 December 2020.

## **5. Solar Off-grid Entrepreneur (30 hrs)**

MNRE schemes and state wise subsidy process

Practice: Identify and specify different types of Solar PV Off grid products

Cost of different solar off grid systems components

Practice: Costing sheet preparation

Selection criteria of suitable components

Practice: Proposal preparation with payment terms and condition

Assessment of business development

Practice: Analysis and assessment of project cost

Economic profile and power consumption trends

Practice: Customer financial strength calculation

Government and private bank funding systems

Practice: Identify the customer requirements for solar home lightning systems

Solar off grid system manufacturers and suppliers

Right equipment should be installed in right place

Attend and resolve customer queries

Entrepreneurship skill



**Text Books:**

1. Rameshwari Pandya, Skill Development and Entrepreneurship in India, 2016.
2. Joseph P. Oconneor, Off Grid Solar, Second edition, Old Sequoia Publishing, 2016.
3. Poornima Charantimath, Entrepreneurship Development and small Business Enterprises, Third edition, Pearson, 2018.

**Reference Books:**

1. C. S. Solanki: Solar Photovoltaic – Fundamentals, Technologies and Applications, PHI Learning Pvt. Ltd., 2011.
1. Michael Boxwell -- Solar Electricity Handbook - 2014 Edition: A Simple Practical Guide to Solar Energy.