Bachelor of Science (Honours) Chemistry under CBCS

PATNA UNIVERSITY, PATNA

Programme Code:

Programme Outcomes

At the completion of the programme, students will attain the ability to:

PO1: : understand the complete idea of periodic table for the systematic study of elements which is essential for the knowledge of various type of compounds.
PO2: develop an idea of spectral properties of covalent molecules and complex compounds.
PO3: understand the quantum mechanical approach of atoms/ molecules .
PO4: understand the structure of various complex molecules including their medicinal properties

Programme Specific Outcomes

At the completion of the programme, students will attain the ability to:

PSO1: visualize the connection between atoms and molecular structure .
PSO2: understand the basics related with the extraction of metals and preparation of their compounds in which some of them are beneficial for mankind .
PSO3: understand the various physical and chemical equilibria effecting the natural processes.
PSO4: skill themselves with the practical approach of inorganic/organic analysis .They will be trained in the preparation of some organic compounds as well as complex compounds.

Course Structure

Semester – I

Sl. No.	Course Code	Name of the Course	Type of Course	L-T-P	Credit	Marks
1		Inorganic Chemistry I: Atomic Structure & Chemical Bonding(Th)	CC-1 (Th)	4-1-0	4	100
2		Inorganic Chemistry I: (P)	CC-1 (P)	0-0-6	2	100
3		Physical Chemistry I: States of Matter & Ionic Equilibrium (Th)	CC-2 (Th)	4-1-0	4	100
4		Physical Chemistry I: States of Matter & Ionic Equilibrium (P)	CC-2 (P)	0-0-6	2	100
5		English Communication/MIL	AECC- 1	2-1-0	2	100
6		Generic Elective- 1 (Th)	GE- 1 (Th)	4-1-0	4	100
7		Generic Elective- 1 (P)	GE- 1 (P)	0-0-6	2	100
Total credit - 20						

Semester – II

Sl. No.	Course Code	Name of the Course	Type of Course	L-T-P	Credit	Marks
1		Organic Chemistry I: Basics and Hydrocarbons (Th)	CC-3 (Th)	4-1-0	4	100
2		Organic Chemistry I: Basics and Hydrocarbons (P)	CC-3 (P)	0-0-6	2	100
3		Physical Chemistry II: Chemical Thermodynamics and its Applications (Th)	CC-4 (Th)	4-1-0	4	100
4		Physical Chemistry II: Chemical Thermodynamics and its Applications (P)	CC-4 (P)	0-0-6	2	100
5		Environmental Science	AECC- 2	2-1-0	2	100
6		Generic Elective- 2 (Th)	GE- 2 (Th)	4-1-0	4	100
7		Generic Elective- 2 (P)	GE- 2 (P)	0-0-6	2	100
Total credit - 20						

Semester – III

Sl. No.	Course Code	Name of the Course	Type of Course	L-T-P	Credit	Marks
1		Inorganic Chemistry II: s- and p-Block Elements (Th)	CC-5 (Th)	4-1-0	4	100
2		Inorganic Chemistry II: s- and p-Block Elements (P)	CC-5 (P)	0-0-4	2	100
3		Organic Chemistry II: Oxygen Containing Functional Groups (Th)	CC-6 (Th)	4-1-0	4	100
4		Organic Chemistry II: Oxygen Containing Functional Groups (P)	CC-6 (P)	0-0-4	2	100
5		Physical Chemistry III: Phase Equilibria and Electrochemical Cells (Th)	CC-7 (Th)	4-1-0	4	100
6		Physical Chemistry III: Phase Equilibria and Electrochemical Cells (P)	CC-7 (P)	0-0-4	2	100
7		Skill Enhancement Course- 1	SEC- 1	2-0-0	2	100
8		Generic Elective- 3 (Th)	GE- 3 (Th)	4-1-0	4	100
9		Generic Elective- 3 (P)	GE- 3 (P)	0-0-4	2	100
Total credit - 26						

Semester – IV

Sl. No.	Course Code	Name of the Course	Type of Course	L-T-P	Credit	Marks
1		Inorganic Chemistry III: Coordination Chemistry (Th)	CC-8 (Th)	4-1-0	4	100
2		Inorganic Chemistry III: Coordination Chemistry (P)	CC-8 (P)	0-0-4	2	100
3		Organic Chemistry III: Heterocyclic Chemistry (Th)	CC-9 (Th)	4-1-0	4	100
4		Organic Chemistry III: Heterocyclic Chemistry (P)	CC-9 (P)	0-0-4	2	100

5		Physical Chemistry IV: Conductance & Chemical Kinetics (Th)	CC-10 (Th)	4-1-0	4	100
6		Physical Chemistry IV: Conductance & Chemical Kinetics (P)	CC-10 (P)	0-0-4	2	100
7		Skill Enhancement Course- 2	SEC- 2	2-0-0	2	100
8		Generic Elective- 4 (Th)	GE- 4 (Th)	4-1-0	4	100
9		Generic Elective- 4 (P)	GE- 4 (P)	0-0-4	2	100
Total credit - 26						

Semester – V

Sl. No.	Course Code	Name of the Course	Type of Course	L-T-P	Credit	Marks
1		Organic Chemistry IV: Biomolecules (Th)	CC-11 (Th)	4-1-0	4	100
2		Organic Chemistry IV: Biomolecules (P)	CC-11 (P)	0-0-4	2	100
3		Physical Chemistry V: Quantum Chemistry & Spectroscopy (Th)	CC-12 (Th)	4-1-0	4	100
4		Physical Chemistry V: Quantum Chemistry & Spectroscopy (P)	CC-12 (P)	0-0-4	2	100
5		Discipline Specific Elective- 1 (Th)	DSE- 1 (Th)	4-1-0	4	100
6		Discipline Specific Elective- 1 (P)	DSE- 1 (P)	0-0-4	2	100
7		Discipline Specific Elective- 2 (Th)	DSE- 2 (Th)	4-1-0	4	100
8		Discipline Specific Elective- 2 (P)	DSE- 2 (P)	0-0-4	2	100
Total credit - 24						

Semester – VI

Sl. No.	Course Code	Name of the Course	Type of Course	L-T-P	Credit	Marks
1		Inorganic Chemistry IV: Organometallic Chemistry (Th)	CC-13 (Th)	4-1-0	4	100
2		Inorganic Chemistry IV: (P)	CC-13 (P)	0-0-4	2	100
3		Organic Chemistry V: Spectroscopy (Th)	CC-14 (Th)	4-1-0	4	100
4		Organic Chemistry V: Spectroscopy (P)	CC-14 (P)	0-0-4	2	100
5		Discipline Specific Elective- 3 (Th)	DSE- 3 (Th)	4-1-0	4	100
6		Discipline Specific Elective- 3 (P)	DSE- 3 (P)	0-0-4	2	100
7		Discipline Specific Elective- 4 (Project/Dissertation)	DSE- 4	0-1-6	6	100
Total credit - 24						

*L/T/P: number of classes per week

DSE/GE may either carry 6 credit, i.e., *Theory (4 credit) + Practical (2 credit) format*
Or
Consolidated (6 credit) for Theory only

Discipline Specific Elective Course (DSE):

Course name	L-T-P
1. Novel Inorganic Solids 2. Inorganic Materials of Industrial Importance 3. Applications of Computers in Chemistry 4. Analytical Methods in Chemistry 5. Molecular Modelling & Drug Design 6. Organometallics, Bioinorganic chemistry, Polynuclear hydrocarbons 7. Polymer Chemistry 8. Green Chemistry 9. Industrial Chemicals & Environment 10. Instrumental Methods of Analysis Dissertation/Project	

Generic Elective (GE):

For Chemistry Students		For Other Students	
Course name	L-T-P	Course name	L-T-P
		1. Atomic Structure, Bonding, General Organic Chemistry & Aliphatic Hydrocarbons 2. Chemical Energetics, Equilibria & Functional Group Organic Chemistry-I 3. Solutions, Phase Equilibrium, Conductance, Electrochemistry & Functional Group Organic Chemistry-II 4. Chemistry of s- and p-block elements, States of matter and Chemical Kinetics 5. Chemistry of d-block elements, Quantum Chemistry and Spectroscopy 6. Organometallics, Bioinorganic chemistry, Polynuclear hydrocarbons and UV, IR Spectroscopy Molecules of life	

Skill Enhancement courses (SEC):

1. IT Skills for Chemists
2. Basic Analytical Chemistry
3. Chemical Technology & Society
4. Business Skills for Chemists
5. Intellectual Property Rights
6. Analytical Clinical Biochemistry
7. Green Methods in Chemistry
8. Pharmaceutical Chemistry
9. Chemistry of Cosmetics & Perfumes
10. Pesticide Chemistry Fuel Chemistry

SEMESTER – I

CC1 : Inorganic Chemistry I Atomic Structure and Chemical Bonding

Course Outcomes

After the completion of the course, the students will be able to understand-

CO1 : the quantum mechanical model of an atom including the related various principles.

CO2 : the complete periodic table and can easily explain the various periodic properties.

CO3 : the principles of bonding as well as shapes and structure of covalent molecules.

CO4 : the term electrode potential and also get idea about volumetric analysis possible in normal chemical laboratory.

CC1 : Inorganic Chemistry I Atomic Structure and Chemical Bonding (Theory: 4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Atomic Structure :** Bohr's Theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrodinger's wave equation, significance of 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 orbitals. Contour boundary and probability diagrams. Pauli Exclusions Principle, Hunds Rule of maximum multiplicity, Aufbau's principle and its limitations, Variations of orbital energy with atomic number.	12
2	**Periodicity of Elements:** S, p, d, f block elements, the long form of periodic table. Detailed discussion of the following properties of the elements, with reference to s and p-block. (a) Effective nuclear charge, shielding or screening effect, Slater rules, variations of effective nuclear charge in periodic table. (b) Atomic radii (Vander Waals) (c) Ionic and crystal radii. (d) Covalent radii (octahedral and tetrahedral) (e) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy. Applications of ionization enthalpy. (f) Electron gain enthalpy, trends of electron gain enthalpy. (g) Electronegativity, Pauling's Mullikens, Allerd Rachow's and Mulliken-Jaffe's electronegativity scales. Variations of electronegativity with bond order, partial charge, hybridization, group electronegativity. Sanderson's electron density ratio.	12
3	**Chemical Bonding:** (i) Ionic bond: General characteristics, types of ions size effects, radius ratio rule and its limitations. Packing of ions in crystals. Born-Lande equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Born-Haber cycle and its application, Solvation enery. (ii) Covalent bond: Lewis structure, Valence Bond Theory (Heitler-London approach). Energetics of hybridization, equivalent and non-equivalent hybrid orbitals. Bent's rule, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules N2, Oxygen, carbon, boron fluorine carbon monoxide, NO, and their ions; hydrogen chloride, berrylium fluoride, carbon dioxide, (idea of s-p mixing and orbital interaction to be given). Formal charge, Valence shell electro pair repulsion theory (VSEPER), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding (sigma and pi bond approach) and bond lengths. Covalent character in ionic compounds, polarizing power and polaizability. Fajan's rule and consequences of polarization. Ionic character in covalent compounds: Bond moment and dipole moment and electronegativity difference. (iii) Metallic bond: Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids. (iv) Weak Chemical Forces: van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Instantaneous dipole-induced dipole	12

	interactions. Repulsive forces, Hydrogen Bonding (theories of hydrogen bonding, valence bond treatment) Effects of chemical force, melting and boiling points, solubility energetics of dissolution process.	
4	**Oxidation-Reduction:** Redox equations, Standard Electrode Potential and its application to inorganic reactions. Principles involved in volumetric analysis to be carried out in class.	12
	TOTAL	48

Suggested Readings :

1. Advanced Inorganic Chemistry, F.A. Cotton, G. Wilkinson.
2. Concise Inorganic Chemistry, J.D. Lee, Blackwell Science, 2001.
3. Inorganic Chemistry, J.E. Huheey, E.A. Keiter and R.I. Keiter, Pearson Education Asia, 2000.
4. Inorganic Chemistry, ELBS 2nd Edition, D.F. Shriver, P.W. Atkins and C.H. Langford. Oxford University Press 2002.
5. Principles of Inorganic Chemistry. B.R. Puri, L.R. Sharma, Jauhar S.P., S.N. Chand & Co.
6. Inorganic Chemistry, 3rd Edition (ISE) A.G. Sharpe Addison Wesley.

CC1 : Inorganic Chemistry I Atomic Structure and Chemical Bonding

After the end of this practical course , the students will be skilled in

CO1 : the preparation of standard solutions for any experimental use.
CO 2 : handing any type of redox titraion.

CC1 : Inorganic Chemistry I Atomic Structure and Chemical Bonding (Practical : 2 credit)
Practical a. Preparation and dilution of standard solutions:- b. Permangnatometry / dichromatry c. Iodometry / iodimetry

Suggested Readings :

1. Practical inorganic chemistry : Shikha Gulati and J. L . Sharma
2. Practical Chemistry : Dr O .P. Pandey , D.N. Bajpayi & ,Giri.

CC2 : Physical Chemistry I : States of matter and Ionic Equilibrium

Course Outcomes

After the completion of this course, the student will be able to understand:

CO1: The mathematical expressions for different Properties of gas, liquid and solid and understand their physical significance.

CO2: The Crystal structure, and may calculate related properties of cubic systems.

CO3: The concept of ionization of electrolytes with emphasis on weak acid and base and hydrolysis of salt.

CO4: The concepts of pH, pK_w, Buffer Solutions, Solubility Product etc. and their applications in day-to-day life.

CC2 : Physical Chemistry I : States of matter and Ionic Equilibrium (Theory: 4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**States of matter and Ionic Equilibrium** **Gaseous state:** Kinetic molecular model of a gas postulates and concept of an Ideal gas, Derivation of the kinetic gas equation and various gas laws; Maxwell's Distribution of Molecular velocities and its use in evaluating different types of molecular velocities – Most Probable Velocity, Average (Mean) Velocity, Root Mean Square (RMS) Velocity, and Average kinetic energy; Relationship between various molecular velocities; Law of equipartition of energy, degrees of freedom and molecular basis of heat capacities. Viscosity of gases, co-efficient of viscosity and its dependence on temperature and pressure; Collision frequency, Collision diameter and Mean free path; Relationship between mean free path (λ) and co-efficient of viscosity (η), Calculation of collision diameter (σ) from co-efficient of viscosity (η). Behaviour of real gases: Deviations form ideal gas behavior, compressibility factor Z, and its variation with pressure for different gases; Causes of deviation from ideal behaviour. Equation of states for real gases; Van der Waals equation of state, its derivation and application in explaining real gas behaviour, Virial coefficients, calculation of Boyle temperature; Isotherms of real gases and their comparison with van der Waals isotherms, continuity of states, critical state & critical constants, relation between critical constants and van der Waals constants, law of corresponding states.	15
2	**States of matter and Ionic Equilibrium** **Liquid state:** 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. Explanation of cleansing action of detergents. Temperature variation of viscosity of liquids and comparison with that of gases.	09
3	**States of matter and Ionic Equilibrium** **Solid state:** Nature of the solid state, law of constancy of interfacial angles, law of rational indices, miller indices, elementary ideas of symmetry, symmetry elements and symmetry operations, qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices; x-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method; Analysis of powder diffraction patterns of NaCl, CsCl and KCI.	09
4	**States of matter and Ionic Equilibrium** **Ionic equilibria**: Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, dissociation constants of mono and diprotic acids; pH and pOH, pH scale; common ion effect; Salt hydrolysis, calculation of hydrolysis constant, degree of hydrolysis and pH for different salts.	15

	Bufffer solutions; derivation of Henderson equation and its applications; Solubili product of sparingly soluble salts, applications of solubility product princip treatment of acid- base titration curves (calculation of pH at various stages). Theo indicators; selection of indicators and their limitations.	
	TOTAL	48

Suggested Readings :

1. Atkins, P.W.; Paula, J.de.; Atkin's Physical Chemistry; Oxford University Press.
2. Ball, D.W.; Physical Chemistry; Cengage Learning, India.
3. Castellan, G.W; Physical Chemistry; Narosa.
4. Kapoor, K.L.; A Textbook of Physical Chemistry, Vol 1, 6Th Edition; McGraw Hill Education.
5. Puri, Sharma, Pathania; Principles of Physical Chemistry; Vishal Publishing Co.
6. Pahari, S.; Physical Chemistry Vol I & II; New Central Book Agency (P) Ltd.
7. Moore, W.J.; Physical Chemistry, 5th Edition, Longmans Green & Co. Ltd.
8. Glasstone, S.; Textbook of Physical Chemistry; D. Van Nostrand company, New York.

CC2 : Physical Chemistry I : States of matter and Ionic Equilibrium

When the students will finish this practical course , they will be skilled in :-

CO1 :determination of coefficient of viscosity of various type of solutions and also in the determination of the surface tension of the various type of aqueou solutions.

CO2: molecular weight determination by victor mayer method.

CO3: pH dermination of various type of buffer solutions.

CC2 : Physical Chemistry I : States of matter and Ionic Equilibrium
(Practical: 2 credits)

Practical :

Surface tension measurements using Stalagmometer

Determine the surface tension of aqueous solutions by (a) drop number, (b) drop weight method.

Viscosity measurement using Ostwald's viscometer.

1. Determination of co-efficient of viscosity of an unknown aqueous solution.
2. Study of variation of viscosity with different concentration of sugar solutions.

Molecular weight of a volatile compound

Determination of molecular weight of a volatile compound using Victor Meyer's method.

Solid State:

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

pH- metry:

1. Study the effect of addition of HCI/ NaOH on pH to the solutions of acetic acid, sodium acetate and their mixtures.
2. Preparation of buffer solutions of different pH values
   (a) Sodium acetate- acetic acid
   (b) Ammonium chloride-ammonium hydroxide
3. pH metric titration of (a) strong acid with strong base, (b) weak acid with strong base and determination of dissociation constant of a weak acid.

Suggested Readings :

1. Khosla, B.D.; Garg, V.C. & Gulati, A.; Senior Practical Physical Chemistry; R. Chand & Co, New Delhi.
2. Garland, C.W.; Nibler, J.W.; Shoemaker, D.P.; Experiments in physical Chemistry, 8th Edition, McGraw-Hill, New York.
3. Yadav, J. B.; Advanced Practical Physical Chemistry, 32nd Ed; Goel Publishing House.

SEMESTER- II

CC3 : Organic Chemistry-1 : Basics and hydrocarbons

Course Outcomes

After the completion of this course, the student will be able to understand:

CO1: The idea of the shape of the molecules, stereochemistry of the molecules through which they can draw various conclusions related with reactions.

CO2: The stability and reactivity of the species involved in the reactions.

CO3: The aromatic character of the molecules.

CO4: The idea to design some organic synthesis.

CC3 : Organic Chemistry-1 : Basics and hydrocarbons (Theory: 4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Recapitulation of the basics in Organic Chemistry** Nomenclature of branched alkanes and polyfunctional group containing compounds, reactivity table. Effect of Hybridization on the shape and bond strength in organic compounds, Electron displacement effects (Inductive effect electromeric effect, resonance/mesomeric effect, hyper–conjugative effect), Applications of electron displacement effect(relative acid- base strength of organic compounds and relative reactivity of aromatic compounds. Electrophilic and nucleophilic reagents nucleophilicity vs basicity, curley arrow rule, Fission of the bonds, shape and relative stability of carbocations carbanions, free redicals, carbenes. Type of organic reactions :- addition, substitution and elimeination reactional.	12
2	**Streo chemistry** Geometrical isomerism around >C=C<, >C=N-, —N–N– bonds ; cis-trans, Z-E and syn-anti notations in geometrical isomers, properties of geometrical isomers. Fischer, Newmanns and sawhorse projection formulae with their interconversions; chirality/asymmetry, optical activity, optical activity in molecules containing one or more asymmetric carbons, specific rotation enantiomers, distereomers, meso forms, racemic mixture, resolution, relative and absolute configuration of optical isomers.	12
3	**Chemistry of aliphatic Hydrocarbons** Preprations of Alkanes, conversion of functional group containing compounds into alkane, clemensons reduction, Wolf Kisners reduction, Wurtz reaction, -relative reactivity and selectivity in halogenation of alkanes. Preparation of alkenes and alkynes; E1, E2 and E1CB mechanism, Saytzeff's and Hofmann's eliminations. Electrophilic additions: hydrohalogenation, Markownikoffs and antimarkownikoffs additions, acid hydration,oxymercuration-demercuration,Glyoxylation,Ozonolysis. Hydroboration-oxidation; 1,2 and 1,4- additions to conjugated dienes, acidity of alkynes, alkylation of alkynes.	12
4	**Chemistry of cyclic Hydrocarbons** Nomenclature of monocyclic and bicyclic alicyclic compounds,Bayers strain theory ,relative stability of chair, boat and twist boat forms of cyclohexane with their energy level diagram , relative stabity of mono-subsituted cyclohexanes.Aromaticity and Huckels rules with reference to benzenoids cyclocarbocations and cyclocarbanions ,mechanism of electrophilic aromatic substitution in benzene- halogenation, nitration ,sulphonation ,Friedel Crafts alkylation/acylation,energy profile diagrams of these reactions,reactivity of mono-subsituted benzene,directive influence of the functional groups, ortho-para ratio.	12
	TOTAL	48

Suggested Readings :

1. Reaction Mechanism in Organic Chemistry - S.M.Mukherjee and S.P. Singh
2. Organic Chemistry,vol.-1 , I. L .Finar
3. Organic Chemistry – Morrison & Boyd
4. Organic Chemistry : Graham Solomons
5. Oranic Chemistry : Paula Yurkanis Bruice
6. Stereochemistry in Organic Chemistry : D. Nassipuri
7. Stereochemistry- Conformation and Mechanism : P.S.Kalsi.

CC3 : Organic Chemistry-1 : Basics and hydrocarbons

After the end of this practical course ,the students will get basic idea related with:

CO1: The identification of known and unknown organic compounds.

CO2: Preparation of known or unknown compounds.

CC3 : Organic Chemistry-1 : Basics and hydrocarbons (Practical: 2 credits)
Practical : **Simple Laboratory Techniques** 1. Use / selection of solvents for the crystallization of organic solids. 2. Determination of melting points of pure supplied organic solids. 3. Determination of boiling point of liquids having boiling point less than 100°C and having boiling point more than 100°C. 4. Determination of melting point point of impure supllied organic solid. – mixed melting point of two unkown supllied organic solids. 5. Preparation of Sodium extract by using organic compounds (solid & liquid). **Experimental Works** 1. Purify the given organic compounds by using crystallization process. 2. Determine the melting point of Naphthalene, Anthrcene &o-nitrophenol. 3. Determine the melting point of unknown pure supplied organic solids. 4. Determine the melting point of impure organic solid by using mixed melting point technique. 5. Detect nitrogen, Sulphur and halogen in the given organic compound. 6. Organic Preparations : a. oxidise toluene by usung potassium permanganate. b.oxidise benzaldehyde by using any oxidising agent c.convert phenol into nitrophenol or ntrobebenzene into m-dinitrobenzene.

Suggested Readings :

1. Qualitative Organic analysis - Vogel
2. Advance Practical Organic Chemistry- N.K. Vishnoi
3. Practical Organic Chemistry- Bernard Charles Saunders and Frederick george Mann.

CC4 : Physical Chemistry II: Chemical Thermodynamics and Its Applications

Course Outcomes

After the completion of this course, the student will be able to understand :-
CO1 : various thermodynamical terms related with 1st law of thermodynamics.
CO2 : various enthalpy of transformations and can easily understand Kirchoff's law.
CO3 : entropy changes , Gibbs free energy change , partial molal quantity, spontaneous process.
CO4 : the 2nd and 3rd law of thermodynamics.

CC4 : Physical Chemistry II: Chemical Thermodynamics and Its Applications (Theory: 4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Thermodynamics-I:** Definition of thermodynamics terms: System, Surroundings, Types of systems, intensive and extensive properties, State and path functions, Thermodynamics process, Concepts of heat and work. First law of Thermodynamics-Statements, Definition of internal energy and enthalpy, Heat capacities at constant volume and pressure and their relationship, Joule's law, Joule-Thomson coefficient and inversion temperature. Calculation of w, q, dU & dH for the expansion of ideal gases under isothermal and adiabatic conditions for reversible process.	12
2	**Thermochemistry:** Standard state, Standard enthalpy of formation, Hess's law of heat summation and its application, Enthalpy of combustion, Enthalpy of neutralization, Bond dissociation energy and its calculation from thermo-chemical data, Temperature dependence of enthalpy, Kirchoff's equation	12
3	**Thermodynamics-II:** Second law of thermodynamics, Need for the law, different statement of the law, Carnet cycle and its efficiency, Carnot theorem, Concept of entropy, Entropy as a function of V&T, P&T, Entropy change in ideal gases and mixing of gases, Gibbs and spontaneity, variation of G and A with P,V and T, Maxwell relation, Thermodynamic equation of state, Third law of thermodynamics, Nernst heat theorem, Statement, concept of residual entropy, Evaluation of absolute entropy from heat capacity data	12
4	**Systems of Variable Composition:** Partial molar quantities, Dependance of Thermodynamic parameters on composition. Gibbs-Duhem equation, Chemical potential of ideal mixtures, Change in Thermodynamic function in mixing of ideal gases.	12
	TOTAL	48

Suggested Readings :

1. Peter, A. & Paula, J. de. Physical Chemistry9th Ed., Oxford University Press (2011).
2. Castellan, G. W. Physical Chemistry4th Ed.,Narosa (2004).
3. Engel, T. & Reid, P. Physical Chemistry3rd Ed., Prentice-Hall (2012).
4. McQuarrie, D. A. & Simon, J. D. Molecular Thermodynamics Viva Books Pvt. Ltd.: New Delhi (2004).
5. Assael, M. J.; Goodwin, A. R. H.; Stamatoudis, M.; Wakeham, W. A. &Will,S. Commonly Asked Questions in Thermodynamics. CRC Press: NY (2011).
6. Levine, I .N. Physical Chemistry 6th Ed., Tata Mc Graw Hill (2010).
7. Metz, C.R. 2000 solved problems in chemistry, Schaum Series (2006)

Reference Books

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

2. Athawale, V. D. & Mathur, P. Experimental Physical Chemistry New Age International: New Delhi (2001).

CC4 : CHEMICAL THERMO-DYNAMICS AND ITS APPLICATION

After the completion of this course, the student will be able to understand :-

CO1 : determination of various type of enthalpy changes in laboratories.

CO2 : determination of the heat capacity of calorimeter

CC4 : CHEMICAL THERMO-DYNAMICS AND ITS APPLICATION (Practical: 2 credits)
Practical : **CHEMICAL THERMO-DYNAMICS AND ITS APPLICATION (P)** 1. Determination of water equivalent of calorimeter. 2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide. 3. Calculation of enthalpy of ionization of ethanoic acid 4. Determine the basicity of a polybasic acid against standard sodium hydroxide solution. 5. Determination of heat of heat of displacement of Cu by Zn from Cu^{2+} salt solution. 6. Determination of enthalpy of hydration of copper sulphate. 7. Study the solubility of Benzoic acid in water and determination of ΔH. 8. Determination of heat capacity of the calorimeter and integral enthalpy(endothermic and exothermic) solution of salts.

SEMESTER – III

CC5 : Inorganic Chemistry II: s, p and d-block elements

Course Outcomes

After the completion of the course, the student will be able to understand:

CO1: The different oxidation states of elements and their complex formation properties

CO2: The ring, cage and polymers of B, Si & P

CO3: How Carry out preparation of inorganic compounds

CO4: The important properties of transition metals such as their oxidation states, color, magnetic properties; use of Latimer diagrams in identifying oxidizing, reducing and disproportioning species

CO5: Knowledge of noble gases, their compounds, shapes, properties and applications

CC5 : Inorganic Chemistry II: s, p and d-block elements (Theory: 4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Chemistry of s- and p-Block Elements** Periodicity in s- and p-block elements with respect to electronic configuration, atomic and ionic size, ionization enthalpy, electronegativity (Pauling, Mulliken, and Alfred-Rochow scales). Inert pair effect, Relative stability of different oxidation states, diagonal relationship and anomalous behaviour of first member of each group. Allotropy and catenation. Complex formation tendency of s and p block elements.	12
2	**Compounds of s-, p-block Elements** Study of the following compounds with emphasis on structure, bonding, preparation, properties and uses: (a) Boron: Boric acid and borates, boron nitrides, borohydrides (diborane) and borazines.	12

	(b) Carbon: Types of carbide, CaC_2, SiC, Al_4C_3 - preparation, properties and uses (c) Silicon: Silicates, Silanes, siloxanes and silicon halides. (d) Nitrogen & Phosphorus: ammonia-manufacture (Haber's process), Oxides and oxoacids of nitrogen and phosphorus. Phosphonitrilic halides {$(PNCl_2)n$ where n = 3 and 4} (Phosphazenes) (e) Sulphur: Sulphuric acid and its properties as dehydrating agent, oxidizing property and action on metals and non-metals. Peroxo acids of sulphur. (f) Halogen: interhalogen compounds, polyhalide ions, pseudohalogens and basic properties of halogens.	
3	**Chemistry of Noble Gases** Occurrence and Isolation, Rationalization of inertness of noble gases, preparation and properties of XeF_2, XeF_4 and XeF_6. Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF_2), shapes of noble gas compounds using VSEPR theory.	12
4	**Transition Elements** General group trends with special reference to electronic configuration, colour, variable valency, magnetic and catalytic properties, and ability to form complexes. Stability of various oxidation states and e.m.f. (Latimer diagrams) Difference between the first, second and third transition series. Chemistry of Cr, Mn, Fe and Co in various oxidation states with special reference to the following compounds: peroxo compounds of chromium, potassium dichromate, potassium permanganate, potassium ferrocyanide, potassium ferricyanide, sodium nitroprusside and sodium cobaltinitrite.	12
	TOTAL	48

Suggested Readings :

1. Lee, J. D., Concise Inorganic Chemistry, 5th Ed., Wiley India (2008).
2. Housecroft, C. E.; Constable, E. C. Chemistry-An Introduction to Organic, Inorganic and Physical Chemistry, 4th Ed., Pearson Education (2010).
3. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., Shriver Atkins's Inorganic Chemistry, 6th Ed., Oxford University Press India (2015).
4. Miessler, G.; Tarr, D. A., Inorganic Chemistry, 3rd Ed., Pearson Education India (2008).
5. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., Inorganic Chemistry: Principles of Structures and Reactivity, 4th Ed., Pearson Education India (2006).
6. Cotton, F. A.; Wilkinson, G.; Gaus, P. L., Basic Inorganic Chemistry, 3rd Ed., Wiley India (2007).
7. Puri, B. R.; Sharma, L. R.; Kalia, K. C., Principles of Inorganic Chemistry, 33rd Ed., Vishal Publishing (2017).

CC5 : Inorganic Chemistry II: s, p and d-block elements

After the end of this practical course the students will be skilled in :-

CO1 : the identification of basic radicals from known and unknown salts.

CO2 : the identification of acid radicals from known and unknown salts.

CC5 : Inorganic Chemistry II: s, p and d-block elements (Practical: 2 credits)
1. Identification of known cataions and anions from the supplied salt. 2. Identification of basic radicals and acid radicals from unknown salt. Determination of basic and acid radicals from binary inorganic mixture.

Suggested Readings :

1. Raj, G., Advanced Practical Inorganic Chemistry, Krishna Prakashan, Meerut (2013).
2. Mendham, J.; Denney, R. C., Barnes, J. D.; Thomas, M.; Sivasankar, B., Vogel's Quantitative Chemical Analysis, 6th Ed., Pearson Education India (2009).

CC6 : Organic Chemistry II: Oxygen Containing Functional Groups

Course Outcomes

After the completion of the course, the student will be able to understand:

CO1: The preparation, properties and reactions of oxygen containing functional groups.
CO2: To draw plausible mechanisms for reactions involving these functional groups.
CO3: The knowledge on various named organic reactions associated with these functional groups.
CO4: The fair idea on fascinating chemistry of epoxides.
CO5: The detection of o-containing functional groups like alcohols, phenols, carbonyl and carboxylic acid group.
CO6: The preparation of various organic compounds by functional group transformations and other common organic reactions.
CO7: The green practices in organic synthesis.

CC6 : Organic Chemistry II: Oxygen Containing Functional Groups (Theory: 4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Alcohols, Phenols, Ethers, and Epoxides** **Alcohols:** Classification and nomenclature and properties Preparation: Preparation of 1^{o}, 2^{o} and 3^{o} alcohols: using substitution reaction, addition reactions, and using Grignard reagent, Ester hydrolysis, Reduction of aldehydes, ketones, carboxylic acid and esters. Reactions: With sodium, HX (Lucas test), esterification, oxidation (with PCC, alk. KMnO4, acidic dichromate, conc. HNO_3). Oppeneauer oxidation Diols: (Upto 6 Carbons) oxidation of diols. Pinacol-Pinacolone rearrangement. **Phenols:** (Phenol case) Classification, nomenclature and properties Preparation: Cumene hydroperoxide method, from diazonium salts. Reactions: Electrophilic substitution: Nitration, halogenation and sulphonation. Fries and Claisen Rearrangement, Kolbe's–Schmidt Reactions, Lederer-Manase reaction, Reimer-Tiemann Reaction, Gattermann-Koch Reaction, Houben–Hoesch Condensation, Schotten – Baumann Reaction. **Ethers and epoxides (aliphatic and aromatic):** Classification, nomenclature and properties Reactions: Cleavage of ethers with HI. Synthesis of epoxides, Acid and base –catalyzed ring opening of epoxides, orientation of ring opening, reactions of Grignard and organolithium reagents with epoxides.	20
2	**Aldehydes and ketones (aliphatic and aromatic)** Structure, reactivity and preparation; nucleophilic additions, Nucleophilic addition-elimination reactions with ammonia derivatives and their mechanisms; mechanisms of Aldol and Benzoin condensation, Knoevenagel condensation, Claisen-Schmidt, Perkin, Cannizzaro and Wittig reaction, Beckmann and Benzil-Benzilic acid rearrangements, haloform reaction and Baeyer Villiger oxidation, α-substitution reactions, oxidations and reductions (Clemmensen, Wolff-Kishner, $LiAlH_4$, $NaBH_4$, MPV and PDC); Addition reactions of unsaturated carbonyl compounds: Michael addition.	10

	Active Methylene Compounds: Keto-enol tautomerism. Preparation and synthetic applications of diethyl malonate and ethyl acetoacetate.	
3	**Carboxylic Acids and their Derivatives** Preparation, physical properties and reactions of monocarboxylic acids. Typical reactions of dicarboxylic acids, hydroxy acids and unsaturated acids: succinic/phthalic, lactic, malic, tartaric, citric, maleic and fumaric acids. Preparation and reactions of acid chlorides, anhydrides, esters and amides; Mechanism of acidic and alkaline hydrolysis of esters, Claisen condensation, Dieckmann and Reformatsky reactions, Hofmann bromamide degradation and Curtius rearrangement.	09
4	**Carbohydrates** Classification, and General Properties, Glucose and Fructose (open chain and cyclic structure), Determination of configuration of monosaccharides, absolute configuration of Glucose and Fructose, Mutarotation, ascending and descending in monosaccharides. Structure of disacharrides (sucrose, cellobiose, maltose, lactose) and polysacharrides (starch and cellulose) excluding their structure elucidation.	09
	TOTAL	48

Suggested Readings :

1. Greeves, N.; Clayden, J.; Warren, S., Organic Chemistry, 2nd Ed., Oxford University, Press India (2014).
2. Sykes, P., A Guidebook to Mechanism in Organic Chemistry, 6th Ed., Pearson Education India (2003)
3. Ghosh, S. K., Advanced General Organic Chemistry, Part-I & Part-II, 3rd Ed., New Central Book Agency (2010).
4. Bhal, B. S.; Bhal, A., A Textbook of Organic Chemistry, 22nd Ed., S. Chand and Company (2016).
5. Sengupta, S., Basic Stereochemistry of Organic Molecules, 2nd Ed., Oxford University Press India (2018).
6. Finar, I. L. Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).

CC6 : Organic Chemistry II: Oxygen Containing Functional Groups

When the students will finish this practical course , they will be skilled in :-

CO1 : acetylation and benzoylation of vorious functional groups present in organic compounds.

CO2: oxime formation , hydrazone formation, semicarbazone formation , iodoform test and in the bromination of phenols.

CO3 :oxidation of alcohols and reduction of nitro compounds .They can easily handle the hydrolysis of esters and amides.

CO4 : Aldol condensation by conventional and green methods.

CC6 : Organic Chemistry II: Oxygen Containing Functional Groups (Practical: 2 credits)
(a) Acetylation of one of the following compounds: phenols (β -naphthol, vanillin, salicylic acid) by any one method: Using conventional method/ Using green approach (b) Benzolyation of one of the following amines (aniline, o-, m-, p- toluidines and o-, m, p-anisidine) and one of the following phenols (β -naphthol, resorcinol, p- cresol) by Schotten-Baumann reaction. (c) Oxime and 2,4-dinitrophenylhydrazone of aldehyde/ketone (d) Oxidation of ethanol/ isopropanol (Iodoform reaction). (e) Semicarbazone of any one of the following compounds: acetone, ethyl methyl ketone, cyclohexanone, benzaldehyde. (f) Aldol condensation using either conventional or green method. (g) S-Benzylisothiouronium chloride from thiourea and benzyl chloride. (h) Reduction of p-nitrobenzaldehyde/ m-nitrobenzaldehyde by sodium borohydride. (i) Bromination of Phenol Hydrolysis of amides and esters.

Suggested Readings :

1. Agarwal, O. P., Advanced Practical Organic Chemistry, Krishna Prakashan, Meerut (2014).
2. Ahluwalia, V. K.; Aggarwal, R., Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, Universities Press (2000).
3. Furniss, B. S.; Hannafold, A. J.; Smith, P. W. G.; Tatchell, A. R., Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Pearson Education India (2003).
4. Clarke, H. T., A Handbook of Organic Analysis: Qualitative and Quantitative, 4th Ed., CBS Publishers India (2007).
5. Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., Textbook of Practical Organic Chemistry, Prentice-Hall, 5th edition, 1996.
6. Mann, F.G. & Saunders, B.C. Practical Organic Chemistry Orient-Longman, 1960.
7. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).

CC7 : Physical Chemistry III: Phase Equilibria and Electrochemical Cells

Course Outcomes

After the completion of the course, the student will be able to:

CO1: Have fair idea on phase equilibrium, phase rule and phase diagram of systems with one to three components.

CO2: Understand Nernst distribution law, its applications in extraction processes and limitations.

CO3: Construct phase diagram and to determine critical solution temperature for simple systems practically.

CO4: Understand conductance and conductivity, application of conductance measurement in determining various physical chemistry parameters.

CO5: Understand standard electrode potential of half cells and calculation of EMF of a cell using Nernst equation.

CO6: Apply EMF measurements in determining various parameters like free energy, enthalpy, entropy, equilibrium constants, etc.

CO7: Have basic knowledge on concentration cells with and without transference.

CO8: Learn the principle of potentiometric titration.

CC7 : Physical Chemistry III: Phase Equilibria and Electrochemical Cells (Theory: 4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Phase Equilibrium** Phases, components and degrees of freedom of a system, criteria of phase equilibrium. Gibbs Phase Rule and its thermodynamic derivation. Derivation of Clausius – Clapeyron equation and its importance in phase equilibria. Phase diagrams of one-component systems (water and sulphur) and two component systems involving eutectics, congruent and incongruent melting points (lead-silver, $FeCl_3$ -H_2O and Na-K only). Nernst distribution law and its limitations, thermodynamic derivation. Modification of distribution law to cases of association and dissociation of solute and complex formation. Application of the law in the process of extraction.	12
2	**Conductance** Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes. Kohlrausch law of independent migration of ions. Transference number and its experimental determination using Hittorf and	12

	Moving boundary methods. Ionic mobility. Applications of conductance measurements: determination of degree of ionization of weak electrolyte, solubility and solubility products of sparingly soluble salts, ionic product of water, hydrolysis constant of a salt. Conductometric titrations (only acid-base).	
3	Reversible and irreversible cells. Concept of EMF of a cell. Measurement of EMF of a cell. Nernst equation and its importance. Types of electrodes. Standard electrode potential. Electrochemical series. Thermodynamics of a reversible cell, calculation of thermodynamic properties: ΔG, ΔH and ΔS from EMF data. Calculation of equilibrium constant from EMF data. Concentration cells with transference and without transference. Liquid junction potential and salt bridge. pH determination using hydrogen electrode and quinhydrone electrode. Potentiometric titrations -qualitative treatment (acid-base and oxidation-reduction only).	12
4	Applications of Electrochemical cells Calculation of equilibrium constant from EMF data. Concentration cells with transference and without transference. Liquid junction potential and salt bridge. pH determination using hydrogen electrode and quinhydrone electrode. Potentiometric titrations -qualitative treatment (acid-base and oxidation-reduction only).	12
	TOTAL	48

Suggested Readings :

1. Atkins, P. W.; de Paula, J.; Keeler, J., Physical Chemistry, 11th Ed., Oxford University Press India (2018).
2. Bahl, A.; Bahl, B. S.; Tuli, G. D., Essentials of Physical Chemistry, S. Chand and Company (2014).
3. Negi, A. S.; Anand, S. C., Physical Chemistry, New Age International Publishers (2007).
4. Puri, B. R.; Sharma, L. R.; Pathania, M. S., Principles of Physical Chemistry, 47th Ed., Vishal Publishing (2017).
5. Silbey, R. J.; Alberty, R. A.; Bawendi, M. G., Physical Chemistry, 4th Ed., Wiley India (2006).
6. Rakshit, P. C., Physical Chemistry, Revised Ed. Sarat Book House (2014).
7. Kapoor, K. L., A Textbook of Physical Chemistry: States of Matter and Ions in Solution, Vol. I, 6th Ed., McGraw Hill Education India (2019).

CC7 : Physical Chemistry III: Phase Equilibria and Electrochemical Cells

After this course ,they will be skilled in :

CO1 : the study of equilibria by distribution method .
CO2 : the experiments related with the conductance measurements .
CO3 : the study of phase equilibria diagrams .
CO4 : the potentiometric titrations.

CC7 : Physical Chemistry III: Phase Equilibria and Electrochemical Cells (Practical: 2 credits)
Practical **Distribution** Study of the equilibrium of one of the following reactions by the distribution method: $I_2(aq) + I^-(aq) = I_3^-(aq)$ $Cu^{2+}(aq) + xNH_2(aq) = [Cu(NH_3)_x]^{2+}$ • To study the distribution of iodine between water and CCl_4

- To study the distribution of benzoic acid between benzene and water.

Conductance

a) Determination of cell constant
b) Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.
c) Perform the following conductometric titrations:
   - Strong acid vs. strong base
   - Weak acid vs. strong base

Phase equilibria

a) Construction of the phase diagram of a binary system (simple eutectic) using cooling curves.
b) Determination of the critical solution temperature and composition of the phenol water system and study of the effect of impurities on it.
c) Study of the variation of mutual solubility temperature with concentration for the phenol water system and determination of the critical solubility temperature.

Potentiometry

Perform the following potentiometric titrations:

- Strong acid vs. strong base
- Weak acid vs. strong base

Potassium dichromate vs. Mohr's salt

Suggested Readings :

1. Viswanathan, B.; Raghavan, P. S., Practical Physical Chemistry, Viva Books India (2014).
2. Yadav, J. B., Advanced Practical Physical Chemistry, Krishna Prakashan, Meerut (2015).
3. Khosla, B. D.; Garg, V. C.; Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co., New Delhi (2011).

SEMESTER – IV
CC8 : Co-ordination Chemistry

Course Outcomes

After the completion of the course, the student will be able to:

CO1: Understand the terms, ligand, denticity of ligands, chelate, coordination number and use standard rules to name coordination compounds.

CO2: Discuss the various type s of isomerism possible in such compounds and understand the types of isomerism possible in a metal complexes.

CO3: Use Valence Bond Theo ry to predict the structure and magnetic behavior of metal complexes and understand the terms inner and outer orbital complexes.

CO4: Explain the meaning o f the terms pairing energy, CFSE, high spin and low spin and how CFSE affects thermodynamic properties like lattice enthalpy and hydration enthalpy.

CO5: Explain magnetic prope rties and colour of complexes on the basis of Crystal Field Theory.

CO6: Understand the import ant properties of transition metals the variable oxidation states, Colours, magnetic and catalytic properties.

CC8 : Co-ordination Chemistry (Theory: 4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Coordination Chemistry -I** Molecular addition compounds, double salts and coordination compounds, coordination sphere, coordination number (C.N). oxidation state (O.S.) of the central metal atom Ligands and classification of ligands, chelate, chelating ligands and its stability. Werner's theory of coordination compounds, limitation of Werner's theory, effective atomic number rule (EAN) . Nomenclature of coordination compounds, isomerism in coordination compounds. Valance bond theory (VBT) of coordination compounds.	12
2	**Coordination Chemistry -II**	12

	Limitation of valence bond theory (VBT), crystal field theory (CFT), crystal field splitting of d-orbitals in the octahedral, tetrahedral, tetragonal and square planar complexes. HS and LS – complexes, factors affecting the octahedral splitting enery, spectrochemical series, magnetic properties of transition metal complexes, colour of transition metal complexes. Crystal field stabilization energy (CFSE), variation of octahedral ionic radii, heat of hydration ,lattice energy of bivalent metal ions of the transition metals, crystal structure of spinals.	
3	**Coordination Chemistry -III** (a) Jahn-Teller effect and distortion in octahedral and tetrahedral complexes. Charge transfer spectra (LMCT)and (MLCT). (b) Magnetic properties of tr ansition metal complexes : Types of magnetic behavior, methods of determination of magnetic susceptibility, L-S coupling, correlation of the magnetic moment (Spin only formula) and effective magnetic moment values, quenching of d-orbitals and orbital contribution to magnetic moment, application of magnetic moment data for 3d - series	12
4	**Chemistry of f-block elements** (a) Chemistry of lanthanides (4f- elements): Classification of f-block elements, position of lanthanides in the periodic table , electronic structure, oxidation state , ionic radii and lanthanides contraction, consequence of lanthanides contraction, complex formation, occurrence and isolation of lanthanides, lanthanide compounds. **(b)** Chemistry of actinides (5f- elements): Position of actinides in the periodic table, source of actinides, General features and chemistry of actinides, separation of Np, Pu and Am from U present in spent fuel Comparisons between lanthanides and actinides.	12
	TOTAL	48

Suggested Readings :

1. Selected topics in inorga nic chemisty- Malik, Madan and Tuli
2. Chemisty for degree stu dents- R.L.Madan.
3. Inorganic Chemisty – G ary L. Miessler and Donald A. Tarr.
4. Advanced Inorganic che mistry- F.A. Coton and Wilkinson.
5. Concise Inorganic Chem istry – J.D. Lee.
6. Inorganic Chemistry - P .W. Atkins.
7. Advanced Inorganic Ch emistry – Kalia, Puri and Sharma

CC8 : Co-ordination Chemistry

At the end of this practical course , the students will be trained in :-

CO1 : the preparation of varios complex compounds.

CO2 : the preparation of common Inorganic compounds.

CC8 : Co-ordination Chemistry (Practical: 2 credits)
Practical Preparation of complexes / inorganic compounds, Potash alum[K2

Suggested Readings :

1. Qualitative inorganic chemistry – Vogel
2. Advance practical inorganic chemistry – Gurdeep Raj

CC9 : Organic Chemistry III: Polynuclear Hydrocarbons and nitrogen containing compounds

Course Outcomes

After the completion of the course, the student will have very good idia about :-

CO1 : the chemistry of Polynuclear Hydrocarbons and terpenoids .
CO2 : the name reactions related with amines,nitriles ,isocynides, and diaazo compounds.
CO3 : the chemistry of some common hetrocyclic compounds.
CO4 : the elementry idea about some alkaloids.

CC9 : Organic Chemistry III: Polynuclear Hydrocarbons and nitrogen containing compounds (Theory: 4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Polynuclear hydrocarbons and terpenoids** Nomenclature of polynuclear hydrocarbons, Preparation of Naphthalene, Anthracene and Phenanthrene, electrophilic substitution in Naphthalene, oxidation and reduction of these hydrocarbons, constitution of Naphthalene. Terpenoids, isoprene rule, classification, reactions used in general structural determination of terpenoids.	10
2	**Nitrogen containing compounds: Amines, Nitriles and Isocyanides, diazouium compound.** Relative basic strength of aliphatic and aromatic amines, effect of solvent on basic strength, prepation, separation. (Hinsberg's method) and Identification of primary, secondary and tertiary amines, Carbylamine reaction, Gabriel phthalimide synthesis, Mannich reaction, Hofmann's exhaustive methylation, simple reactions of amines, Eschweiler Clarke methylation, reductions of nitro compound under various conditions. Formation of diazonium salts and their synthetic applications. Diazocoupling reaction, Gomberg reaction, Preparation of nitriles and isonitriles. Important reactions of nitriles and isonitriles. von Ritcher reaction.	15
3	**Heterocyclic compounds** Classification and nomenclature of heterocyclic compounds, aromaticity in 5- & 6-membered ring with one heteroatom. Synthesis of Furan, Thiophene, Pyrrole (Knorr Pyrrole synthesis, Paal Knorr synthesis, Hantzsch synthesis) ,Synthesis of Pyridine (Hantzsch synthesis), reactions of Pyrrole and Pyridine. Structures of Pyrimidine, Quinoline and isoquinoline. Skraup synthesis, Friedlander's synthesis, Knorr Quinoline synthesis, Bischler Napieralski Reaction synthesis of Isoquinoline, Constitution of Quinoline.	15
4	**Alkaloids** Natural occurance, classfication and isolation of alkaloids, reactions used in general structural determination, medicinal activity of the compounds, Emde degradation. Medicinal properties of Nicotine, Quinine, Morphine and Reserpine.	08
	TOTAL	48

Suggested Readings :

1. Morrison R.T., Boyd R.N., (2007) Organic Chemistry, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar I.L., (2014) Organic Chemistry (Volume 1), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Finar I.L., (2014) Organic Chemistry (Volume 2: Stereochemistry and the Chemistry of Natural Products), Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
4. Acheson R.M., (1976), Introduction to the Chemistry of Heterocyclic compounds, John Wiley & Sons.
5. Graham Salomons T.W., Organic Chemistry, John Wiley & Sons, Inc.
6. Kalsi P.S.,(2010), Textbook of Organic Chemistry 1st Ed., New Age International (P) Ltd. Pub.

CC9 : Organic Chemistry III: Polynuclear Hydrocarbons and nitrogen containing compounds

After this practical course ,the students can easily perform :

CO1 : tests related with nitrogen and nitrogen cotaining functional groups.

CO2 :tests related with alkaloids.

CC9 : Organic Chemistry III: Polynuclear Hydrocarbons and nitrogen containing compounds (Practical: 2 credits)
Practical : 1. Detection of nitrogen in orgain compounds . 2. tests of nitro, amino groups . 3. carbayl amine reaction . 4. diazo -coupling reactions . 5. detection of alkaloids . 6. Nitration of Naphthalene.

CC10 : PHYSICAL CHEMISTRY IV SOLUTION AND CHEMICAL KINETICS

Course Outcomes

After the completion of the course, the student can easily understand the:-

CO1 : colligatve properties of different solutions , theoretcal and experimenal measurements of these properties.

CO2 : kinetics of simple reactions and some complex reactions.

CC10 : PHYSICAL CHEMISTRY IV SOLUTION AND CHEMICAL KINETICS (Theory: 4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**DILUTE SOLUTION** Dilute solution, Lowering of vapour pressure, Raoult's law and Henry's law and their applications, Duhemmarguls equation, Ideal and Non ideal solutions, Azeotropes, Maximum and minimum Azeotropes	08
2	**COLLIGATIVE PROPERTIES OF SOLUTIPON** Thermodynamic derivation of colligative properties • Relative lowering of vapour pressure • Elevation of Boiling point • Depression of Freezing points • Osmotic pressure Abnormal Colligative properties, Vant' Hoff Factor, Applications of Colligative properties i9n calculating of Molar mass of solute- Normal , Dissociated, Associated. ,Experimental methods for the detemination of various colliagative properties .	20
3	**KINETICS OF ELEMENTARY REACTIONS** Order and molecularity of a reaction, Rate laws in term of advancement of a reaction, Differential and integrated form of rate expressions upto second order of reaction, methods of determination of order of reactions, Temp dependance of reaction rate, Arrhenius equation, Activation energy, Collision theory of reaction rate , Qualitative treatment of the theory of the absolute reaction rates.	10
4	**KINETICS OF COMPLEX REACTIONS** Integrated rate expression upto First order only for the 1. Opposing reactions	10

	2. Parallel reactions and Consecutive reactions(Steady state approximation in reaction mechanism.	
	TOTAL	48

Suggested Readings :

1. Physical Chemistry : P.W. Atkins (ELBS)
2. Comprehensive Physical Chemistry : Hemant Snehi
3. Theoretical Physical Chemistry : Gladstone
4. Physical Chemistry: G.M. Barrow.
5. Modern Electrochemistry : JOM Bakris and A.K.N. Reddy
6. Text Books of Polymer Science : F.W. Billmayer Jr
7. Advanced Physical Chemistry : Gurdeep Raj

CC10 : PHYSICAL CHEMISTRY IV SOLUTION AND CHEMICAL KINETICS

At the end of this practical course the students will be skilled in :-

CO1 : molecular weight determination by elevation in boiling point and depression in freezing point methods.

CO2 : the determination of the velocity constants of the hydrolsis of esters and inversion of cane sugar .

CC10 : PHYSICAL CHEMISTRY IV SOLUTION AND CHEMICAL KINETICS
(Practical: 2 credits)

Practical :

SOLUTION

1. To determine the molecular weight of a non volatile substances(Urea) by Landsberger's method.
2. To find the molecular weight of a non volatile solute(Urea) by Beckmann f. p. depression method.
3. To determine the viscosity of a liquid or solution
4. To determine the surface tension of alcohol water mixture and hence to find out the composition of an unknown mixture.

CHEMICAL KINECTICS

1. To determine the velocity constant of hydrolysis of Methyl Acetate catalysed by HCl.
2. To determine the velocity constant of inversion of cane sugar.
3. To determine the velocity constant of hydrolysis(or saponiofication) of Ethyl Acetate with NAOH.

Suggested Readings :

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

SEMESTER – V
CC11 : ORGANIC CHEMISTRY – IV

Course Outcomes

After the completion of the course, the student will be able to:

CO1: Genetic materials involved in living biosystems.
CO2: Physicochemical properties of aminoacids, peptides and proteins.
CO3: Enzymes and their activity as well as some basic idea about Lipids.
CO4: The basics of energetics in biosystems and introduction to some synthetic and naturally occurring pharmaceuticals.

CC11 : ORGANIC CHEMISTRY – IV (Theory: 4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Nucleic Acids** Components of nucleic acids, Nucleosides and nucleotides; Structure andsynthesis of: Adenine, Guanine, Cytosine, Uracil and Thymine.Structure of Polynucleotides and DNA duplex.	10
2	**Amino Acids, Peptides and Proteins** Classification of α-Amino Acids –General methods of Synthesis, ionic properties and reactions. Zwitterions, pKa values, isoelectric point and electrophoresis. Study of peptides: Oligo and polypeptides, features of peptide bonds. Synthesis of peptides using N-protecting, C-protecting and C-activating groups. Solid-phase synthesis. Elementary idea of primary, secondary, tertiary and quarternary structures of proteins.	10
3	**Enzymes and Lipids** Introduction, classification and characteristics of enzymes. Mechanism of enzyme action (taking trypsin as example), factors affecting enzyme action.Specificity of enzyme action.Enzyme inhibitors and their importance, phenomenon of inhibition (competitive, uncompetitive and non-competitive inhibition. Introduction to oils and fats, Hydrogenation and iodine number.	08
4	**Concept of energy in Biosystems and Pharmaceutical compounds** Meaning and applications, Role of ATP in glycolysis during Phosphorylation of glucose, Conversion of glucose-6-phosphate to fructose-6-phosphate, phosphorylation of fructose-6-phosphate, cleavage of fructose-1,6-biphosphate, oxidation of glyceraldehydes 3-phosphate to 1,3-biphosphoglycerate, phosphoryl transfer from biphosphate to ADP, Conversion of 3-phosphoglycerate to 2-phosphoglycerate, dehydration of 2-phosphoglycerate, transfer of the phosphoryl group from phosphoenol pyruvate to ADP and overall energy balance sheet for ATP. Structure, synthesis and therapeutic uses of Paracetamol and Ibuprofen.Medicinal values of curcumin(haldi), azadirachtin (neem) and vitamin C.	20
	TOTAL	48

Suggested Readings :

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.

CC11 : ORGANIC CHEMISTRY – IV

The students will be skilled after this practical course in :-

CO1 : tests of carbohydrates and amino acids.

CO2 : the experiments related with enzymes ,oils and fats.

CC11 : ORGANIC CHEMISTRY – IV (Practical: 2 credits)
Practical : **Laboratory tests for carbohydrates and experimental aspects of amino acids.** 1. Testing carbohydrates by Fehling's solution, Tollen's reagent and Benedict's reagent. 2. Molisch's test, Barfoed test and Seliwanoff test for carbohydrates, Preparation of Osazone derivetives of carbohydrates. 3. Estimation of glycine by Sorenson's formalin method. 4. Study of the titration curve of glycine. **Experiments related to Enzymes, oils and fats.** 1. Study of the action of salivary amylase on starch at optimum conditions. 2. Effect of temperature on the action of salivary amylase. 3. Saponification value of an oil or a fat. 4. Determination of Iodine number of an oil/ fat.

Suggested Readings :

1. Manual of Biochemistry Workshop, 2012, Department of Chemistry, Universityof Delhi.
2. Arthur, I. V. *Quantitative Organic Analysis,* Pearson.
3. Any other laboratory manual available in departmental library as advised by the instructor.

CC12 : PHYSICAL CHEMISTRY V QUANTUM CHEMISTRY & SPECTROSCOPY

Course Outcomes

After the completion of the course, the student will be able understand :-

CO1 :- the postulates of quantum mechanics, Schrondinger's wave equation and its applications

CO2 : the concepts related with the electronic and rotational spectra.

CO3 : the concepts related with vibrational and Raman spectra.

CC12 : PHYSICAL CHEMISTRY V QUANTUM CHEMISTRY & SPECTROSCOPY (Theory: 4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**ELEMENTARY QUANTUM MECHANICS** Postulates of Quantum Mechanics, Quantum Mechanical Operators, Operator properties, Schrodinger wave equation and its importance, physical interpretation of wave function, Heisenberg Uncertainty Principle, Probability distribution function, Nodal properties, Particle in one dimensional box, Particle in three dimension box, Concept of degeneracy, Schrodinger wave equation for Hydrogen atom, Separation into three equation, Hydrogen like wave functions.	12
2	**VALENCE BOND THEORY AND MOLECULAR ORBITAL THEORY** Basic ideas of VBT and MOT, Valence bond model of H_2, Construction of MO's by LCAO/ H_2^+ ion. Physical picture of bonding and antibonding wave functions, Concept of σ, σ^*, π, π^* orbitals, comparison between VBT and MOT. Hybrid orbitals SP,SP^2,SP^3.Calculation of coefficients of atomic orbitals used in this hybrid orbitals.	12
3	**ROTATIONAL AND ELECTRONIC SPECTRUM** Energy level of a rigid rotor, selection rules, spectral intensity, distribution using population distribution, determination of bond length,qualitative description of non-rigid rotor, isotope effect.	12

	Franck-Condon principle electronic transitions, singlet and triplet states, concept of potential energy curves for bonding and anti-bonding molecular orbitals.Fluorescenceand phosphorescence.	
4	**VIBRATIONAL AND RAMAN SPECTROSCOPY** Energy levels of simple harmonic oscillator, selection rules, pure vibrational spectrum, determination of force constants, relation of force constants with bond energy, effect of anharmonic motion, idea of vibrational frequencies of different functional groups, overtones, modes of vibration, vibrational-rotational spectrum, P, Q, R branches. Raman spectrum, concept of polarizability, vibrational Raman spectra, stocks and anti-stocks lines, their intensity difference.	12
	TOTAL	48

Suggested Readings :

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

CC12 : PHYSICAL CHEMISTRY V QUANTUM CHEMISTRY & SPECTROSCOPY

After the end of this practical course ,the student will be skilled :-

CO1 : in doing experiments related with Lamberts Beers law and in the the dtermination of of dissociation constant of an indicator, Phenolphthalein.

CO2 : in handling the UV visisible spectrometer.

CC12 : PHYSICAL CHEMISTRY V QUANTUM CHEMISTRY & SPECTROSCOPY (Practical: 2 credits)
Practical : **QUANTUM CHEMISTRY (P)** 1. Verify Lambert-Beer's law and determine the concentration of CuSO4/KMnO4 in a solution of unknown concentration. 2. Determine the concentrations of KMnO4 and K2Cr2O7 in a mixture. 3. Study the kinetics of iodination of propanone in acidic medium. 4. Determine the dissociation constant of an indicator (phenolphthalein). **SPECTROSCOPY (P)** 1. Study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) and determine the λ_{max} values. 2. Study the pH-dependence of the UV-Vis spectrum (200- 500 nm) of $K_2Cr_2O_7$.

Suggested Readings :

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

SEMESTER – VI

CC13 : Inorganic Chemistry IV: Organometallic Chemistry

Course Outcomes

After the completion of the course, the student will be able to understand the :

CO1 : nomenclature and classification of Organometallic compounds .
CO2 : properties of metal carbonyls incuding their structures.
CO3 :the methods related with the preparation of Organometallics.
CO4 : calalytic properties and biological properties of Organometallics.

CC13 : Inorganic Chemistry IV: Organometallic Chemistry (Theory: 4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Organometallic Chemistry- I** Definition, Nomenclature and Classification of Organometallic com- pounds. Concept of Hapticity.	08
2	**Organometallic Chemistry- II** Metal carbonyls: EAN rule and 18 electron rule applied to Metal Carbonyls, Classification, Preparation, Properties and Bonding of Metal Carbon- yls, π-acceptor behaviour of CO, Synergic effect, Use of IR spectra of Metal Carbonyls, Structure of Mononuclear, Binuclear and Polynuclear metal carbonyls.	10
3	**Organometallic Chemistry- III** General methods of preparation and properties of organometallic com- pounds. Preparation, properties, bonding and applications of alkyls and aryls of Li, Al, Hg, Sn, Ti. Concept of Multicentre bonding in above examples.	10
4	**Organometallic Chemistry- IV** A brief account of Metalethylenic and Metal-acetylene complexes. Zeisse's salt – Preparation, properties, bonding and synergic effect. Ferrocene: Preparation, Reactions, Structure and Aromaticity, Comparison of aromaticity and reactivity with that of benzene.	10
5	**Organometallic Chemistry- V** Catalytic processes of Organometallic Compounds (brief account): Carbonylation, Hydroformylation, Homogeneous Hydrogenation and Hydrogenation. Biological applications of Metal complexes: Metalloporphyrins, Haemoglobin, Myoglobin, Chlorophyll and Vitamin-12.	10
	TOTAL	48

Suggested Readings :

1. Organometallic Chemistry: Gurdeep Chatwal and M. S. Yadav – Himalaya Publish- ing House.
2. Selected Topics in Inorganic Chemistry, by Dr. Wahid U. Malik, Dr. G. D. Tuli and Dr. R. D. Madan – S Chand Publication.
3. Organometallic Chemistry – R. C. Mehrotra and A. Singh – New Age International Publication.
4. Chemistry for Degree Students – B. Sc. Third Year – by Dr. R. D. Madan- S Chand Publication.
5. General Inorganic Chemistry (Vol-II) – by Bidhan Chandra Roy and Satyanarayan Das – NCBA
6. Miessler, G.; Tarr, D. A., Inorganic Chemistry, 3rd Ed., Pearson Education India

CC13 : Inorganic Chemistry IV: Organometallic Chemistry

After the completion of the course, the student will be able to:

CO1 : understand the use of paper chromatography.

CO2 : understand the use of thin layer chromatography.

CC13 : Inorganic Chemistry IV: Organometallic Chemistry (Practical: 2 credits)
Practical : 1.Experiments related with paper chromatography a. Seperation of a mixture of two amino acids by ascending and horizontal paper chromatography. b.seperation of a mixture of two sugars by ascending paper chromatography. cTo separate and identify the metal ions of group 1 from the analytical table. D.To d.separate and identify the metal ions of group 3 of the analytical table. e.To identify the number of components present in a given solutions. 2. To determine the biological oxygen demand from the supplied water sample. 3. To estimate the percentage of nitrogen in given sample of food stuff by Kjeldahl method. 4. To handle the experiments related with thin layer chromatography.-seperation of amixture of o- and p-nitrophenol or o- and p-aminophenol by thin layer chromatography.

Practical :

1. Pratical chromatography – S. Chand & Company.
2. Analytical chemistry – S. Chand & Company

CC14 : ORGANIC SPECTROSCOPY

Course Outcomes

After the completion of the course, the student will be able to:

CO1: Understand structure and properties of different N containing functional groups like amines, nitro, nitriles & isonitries and benzene diazonium chloride and the synthetic application of benzene diazonium chloride.

CO2: Comprehend the Polynuclear Hydrocarbon Structure elucidation and properties of different polynuclear hydrocarbons like naphthalene and anthracene.

CO3: Analyse the different synthetic methods for synthesis of different heterocyclic compounds and application of these methods for the preparation of specific groups of heterocyclic system and the mechanism of different chemical reactions. To understand its wide applications in diverse areas such as dyes, photo sensitizers, co-ordination compounds, etc.

CO4: Synthesis and structure of different alkaloids and terpenes and their medicinal importance.

CC14 : ORGANIC SPECTROSCOPY (Theory: 4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Infrared(IR) absorption Spectroscopy** Introduction :- Origin and spectrum of electromagnetic radiation, Absorption and Emission Spectra. Infrared spectroscopy –molecular vibrations, Degree of freedom, Measurement of IR Spectrum, Functional group and Finger Print region. Factors affecting position andintensityofIRbands,Hooke's law, selection rules, characteristic absorptions of various functional groups, Interpretation of I.R. spectra of simple organic compounds.	18
2	**Ultraviolet(U.V.) absorption spectroscopy** Ultraviolet absorption spectroscopy :- Absorption laws (Beer – Lambert's law) Types of electronic transitions, molar absorption coefficient, selection rules, Analysis and measurement of UV spectra, concept of chromophore, Auxochrome. Bathochromic, hypsochromic, hyperchromic	15

	and hypochromic shifts. Wood-ward's rule for calculation of λmax, U.V. spectra of conjugated enes and enones.	
3	**Nuclear magnetic resonance (NMR) spectroscopy :-** Principle of Nuclear magnetic resonance (^{1}H-PMR) spectroscopy, shielding and deshielding effect, chemical shift. Number position, area and intensity of NMR signals of organic compounds. Splitting of signals, spin-spin coupling and coupling constant.	15
	TOTAL	48

Reading List :

1. Organic Chemistry – Morrison and Boyyd
2. Organic spectroscopy : Y .R. Sharma.

CC14 : SPECTROSCOPY

After the completion of the course, the student will be able to:

CO1 : will get idea about different spectrometer.

CO2 : interpretation of IR, UV and NMR graphs for the elucidation of simple molecular structures.

CC14 : SPECTROSCOPY (Practical: 2 credits)
Practical : **IR, UV, NMR spectrophotometers** A. Basic features and principles of different spectrophotometers. B. Working system of different spectrophotometers. C. Interpretation of functional groups and skeletal structure of simple compounds by analysis of given IR, UV and HMR spectrographs. Structure elucidation of simple organic compounds through IR, UV and NMR spectroscopic technique.

Discipline Specific Elective (DSE)

SEMESTER – V

DSE1 : Novel Inorganic Solids

Course Outcomes

After the completion of the course, the student will be able to:

CO1: Understand the mechanism of solid-state synthesis.
CO2: Explain about the different characterization techniques and their principle.
CO3: Understand the concept of nanomaterials, their synthesis and properties.
CO4: Explain the mechanism of growth of self-assembled nanostructures.
CO5: Appreciate the existence of bioinorganic nanomaterials.
CO6: Explain the importance of composites, conducting polymers and their applications.
CO7: Understand the usage of solid materials in various instruments, batteries, etc. which would help them to appreciate the real life importance of these materials

DSE1 : Novel Inorganic Solids (Theory: 4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Basic introduction to solid-state chemistry:** Semiconductors, different types of semiconductors and their applications. Conventional heat and beat method, Co-precipitation method, Sol-gel method,	08

	Hydrothermal method, Chemical vapor deposition (CVD), Ion-exchange and Intercalation method.	
2	**Synthesis of inorganic solids:** Powder X-ray Diffraction, UV-visible spectroscopy, Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Fourier-Transform Infrared (FTIR) spectroscopy, Brunauer–Emmett–Teller (BET) surface area analyser, Dynamic Light Scattering (DLS)	08
3	**Characterization techniques of inorganic solids:** Cationic, anionic and mixed solid electrolytes and their applications. Inorganic pigments – coloured, white and black pigments. One-dimensional metals, molecular magnets, inorganic liquid crystals.	08
4	**Nanomaterials:** Overview of nanostructures and nanomaterials, classification, preparation and optical properties of gold and silver metallic nanoparticles, concept of surface plasmon resonance, carbon nanotubes, inorganic nanowires, Bioinorganic nanomaterials, DNA and its nanomaterials, natural and artificial nanomaterials, self-assembled nanostructures, control of nanoarchitecture, one dimensional control.	08
5	**Composite materials:** Introduction, limitations of conventional engineering materials, role of matrix in composites, classification, matrix materials, reinforcements, metal-matrix composites, polymer-matrix composites, fibre-reinforced composites, bio-nanocomposites, environmental effects on composites, applications of composites.	08
6	**Speciality polymers:** Conducting polymers - Introduction, conduction mechanism, polyacetylene, polyparaphenylene, polyanilineand polypyrrole, applications of conducting polymers, ion-exchange resins and their applications. **Ceramic & Refractory:** Introduction, classification, properties, manufacturing and applications of ceramics, refractory and superalloys as examples.	08
	TOTAL	48

Reading List :

1. West, A. R. (2014), Solid State Chemistry and Its Application, Wiley.
2. Smart, L. E.; Moore, E. A., (2012),Solid State Chemistry: An Introduction CRC Press Taylor & Francis.
3. Rao, C. N. R.; Gopalakrishnan, J. (1997),New Direction in Solid State Chemistry, Cambridge University Press.
4. Poole Jr.; Charles P.; Owens, Frank J. (2003), Introduction to Nanotechnology, John Wiley and Sons.

DSE1 : Novel Inorganic Solids (Practical: 2 credits)
Practical : 1. Synthesis of silver nanoparticles by chemical methods and characterization using UV-visible spectrophotometer. 2. Synthesis of silver nanoparticles by green approach methods and characterization using UV-visible spectrophotometer. 3. Preparation of polyaniline and its characterization using UV-visible spectrophotometer. 4. Synthesis of metal sulphide nanoparticles (MnS, CdS, ZnS, CuS, NiO) and characterization using UV- visible spectrophotometer. 5. Intercalation of hydrogen in tungsten trioxide and its conductivity measurement using conductometer. 6. Synthesis of inorganic pigments (PbCrO4, ZnCrO4, Prussian Blue, Malachite).

7. Synthesis of pure ZnO and Cu doped ZnO nanoparticles.
8. Preparation of zeolite A and removal of Mg and Ca ions from water samples quantitatively using zeolite.

Practical:

1. Orbaek, W.; McHale, M.M.; Barron, A. R.; Synthesis and Characterization of Silver Nanoparticles for An Undergraduate Laboratory,J. Chem. Educ. 2015, 92, 339−344.
2. MacDiarmid, G.; Chiang, J.C.; Richter, A.F.; Somasiri, N.L.D.(1987), Polyaniline: Synthesis and Characterization of the Emeraldine Oxidation State by Elemental Analysis, L. Alcaeer (ed.), Conducting Polymers, 105-120, D. Reidel Publishing.
3. Cheng, K.H.; Jacobson, A.J.; Whittingham, M.S. (1981),Hexagonal Tungsten Trioxide and Its Intercalation Chemistry, Solid State Ionics, 5, 1981, 355-358.
4. Ghorbani H.R.; Mehr, F.P; Pazoki, H; Rahmani, B.M.; Synthesis of ZnO Nanoparticles by Precipitation Method, Orient J Chem 2015, 31(2).

DSE2 : Inorganic Materials of Industrial Importance

Course Outcomes

After the completion of the course, the student will be able to:

CO1: Learn the composition and applications of the different kinds of glass.
CO2: Understand glazing of ceramics and the factors affecting their porosity.
CO3: Give the composition of cement and discuss the mechanism of setting of cement.
CO4: Explain the suitability of fertilizers for different kinds of crops and soil.
CO5: Explain the process of formulation of paints and the basic principle behind the protection offered by the surface coatings.
CO6: Explain the principle, working and applications of different batteries.
CO7: List and explain the properties of engineering materials for mechanical construction used in day to day life.
CO8: Explain the synthesis and properties of nano-dimensional materials, various semiconductor and superconductor oxides.

DSE2 : Inorganic Materials of Industrial Importance (Theory: 4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Silicate Industries** Glass: Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, different types of safety glass, borosilicate glass, fluorosilicate glass, coloured glass, photosensitive glass, photochromic glass, glass wool and optical fibre. Ceramics: Brief introduction to types of ceramics. glazing of ceramics. Cement: Manufacture of Portland cement and the setting process, Different types of cements: quick setting cements, eco-friendly cement (slag cement), pozzolana cement.	08
2	**Fertilizers:** Different types of fertilizers (N, P and K). Importance of fertilizers, chemistry involved in the manufacture of the following fertilizers: urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates, superphosphate of lime, potassium chloride and potassium nitrate.	08
3	**Surface Coatings:** Brief introduction to and classification of surface coatings, paints and pigments: formulation, composition and related properties, pigment volume concentration (PVC)and critical pigment volume concentration (CPVC), fillers, thinners, enamels and emulsifying agents. Special	08

	paints: heat retardant, fire retardant, eco-friendly paints, plastic paints, water and oil paints. Preliminary methods for surface preparation, metallic coatings (electrolytic and electroless with reference to chrome plating and nickel plating), metal spraying and anodizing. Contemporary surface coating methods like physical vapor deposition, chemical vapor deposition, galvanising, carburizing, sherardising, boriding, nitriding and cementation.	
4	**Batteries:** Primary and secondary batteries, characteristics of an Ideal Battery, principle, working, applications and comparison of the following batteries: Pb- acid battery, Li-metal batteries, Li-ion batteries, Li-polymer batteries, solid state electrolyte batteries, fuel cells, solar cells and polymer cells.	08
5	**Engineering materials for mechanical construction:** Composition, mechanical and fabricating characteristics and applications of various types of cast irons, plain carbon and alloy steels, copper, aluminum and their alloys like duralumin, brasses and bronzes cutting tool materials, superalloys, thermoplastics, thermosets and composite materials.	08
6	**Nano dimensional materials** Introduction to zero, one and two-dimensional nanomaterial: Synthesis, properties and applications of fullerenes, carbon nanotubes, carbon fibres, semiconducting and superconducting oxides..	08
	TOTAL	48

Suggested Readings :

1. West, A. R. (2014),Solid State Chemistry and Its Application, Wiley Smart, L. E.; Moore, E. A. (2012),Solid State Chemistry An Introduction, CRC Press Taylor & Francis.
2. Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A.(2010),Shriver and Atkins Inorganic Chemistry, W. H. Freeman and Company.
3. Kent, J. A. (ed) (1997),Riegel's Handbook of Industrial Chemistry, CBS Publishers, New Delhi.
4. Poole Jr.; Charles P.; Owens, Frank J.(2003), Introduction to Nanotechnology, John Wiley and Sons.

Additional Resources:

1. Kingery, W. D.; Bowen H. K.; Uhlmann, D. R. (1976),Introduction to Ceramics, Wiley Publishers, New Delhi.
2. Gopalan, R. Venkappayya, D.; Nagarajan, S. (2004),Engineering Chemistry, Vikas Publications.

DSE2 : Inorganic materials of industrial importance
(Practical: 2 credits)

Practical :

1. Detection of constituents of Ammonium Sulphate fertilizer (Ammonium and Sulphate ions) by qualitative analysis and determine its free acidity.
2. Detection of constituents of CAN fertilizer (Calcium, Ammonium and Nitrate ions) fertilizer and estimation of Calcium content.
3. Detection of constituents of Superphosphate fertilizer (Calcium and Phosphate ions) and estimation of phosphoric acid content.
4. Detection of constituents of Dolomite (Calcium, Magnesium and carbonate ions) and determination of composition of Dolomite (Complexometric titration).
5. Analysis of (Cu, Ni) in alloy or synthetic samples (Multiple methods involving Complexometry, Gravimetry and Spectrophotometry).
6. Analysis of (Cu, Zn) in alloy or synthetic samples (Multiple methods involving Iodometry, Complexometry and Potentiometry).
7. Synthesis of pure ZnO and Cu doped ZnO nanoparticles.

8. Synthesis of silver nanoparticles by green and chemical approach methods and its characterization using UV-visible spectrophotometer.

Practical:

1. Svehla, G.(1996),Vogel's Qualitative Inorganic Analysis, Prentice Hall.
2. Banewicz, J. J.; Kenner, C.T. Determination of Calcium and Magnesium in Limestones and Dolomites, Anal. Chem., 1952, 24 (7), 1186–1187.
3. Ghorbani, H. R.; Mehr, F.P.; Pazoki, H.; Rahmani B. M. Synthesis of ZnO Nanoparticles by Precipitation Method. Orient J Chem 2015;31(2).
4. Orbaek, W.; McHale, M.M.; Barron, A.R. Synthesis and characterization of silver nanoparticles for an undergraduate laboratory, J. Chem. Educ. 2015, 92, 339−344.

SEMESTER – VI

DSE3 : Applications of Computers in Chemistry

Course Outcomes

After the completion of the course, the student will be able to:

CO1: Have knowledge of most commonly used commands and library functions used in QBASIC programming.

CO2: Develop algorithm to solve problems and write corresponding programs in BASIC for performing calculations involved in laboratory experiments and research work.

CO3: Use various spreadsheet software to perform theoretical calculations and plot graphs

DSE3 : Applications of Computers in Chemistry (Theory:4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Basic Computer system (in brief)** Hardware and Software; Input devices, Storage devices, Output devices, Central Processing Unit (Control Unit and Arithmetic Logic Unit); Number system (Binary, Octal and Hexadecimal Operating System); Computer Codes (BCD and ASCII); Numeric/String constants and variables. Operating Systems (DOS, WINDOWS, and Linux); Software languages: Low level and High Level languages (Machine language, Assembly language; QBASIC, FORTRAN and C++); Compiled versus interpreted languages. Debugging Software Products (Office, chemsketch, scilab, matlab, and hyperchem), internet application.	20
2	Computer Programming Language- QBASIC, (for solving some of the basic and complicated chemistry problems). QB4 version of QBASIC can be used. Programming Language – QBASIC; arithmetic expressions, hierarchy of operations, inbuilt functions. Syntax and use of the following QBASIC commands: INPUT and PRINT; GOTO, If, ELSEIF, THEN and END IF ; FOR and NEXT; Library Functions (ABS, ASC, CHR$, EXP,INT, LOG, RND, SQR,TAB and trigonometric Functions), DIM, READ, DATA, REM, RESTORE, DEF FNR, GOSUB, RETURN, SCREEN, VIEW, WINDOW, LINE, CIRCLE, LOCATE, PSET Simple programs using above mentioned commands. Solution of quadratic equation, polynomial equations (formula, iteration, Newton – Raphson methods, binary bisection and Regula Falsi); Numerical differential, Numerical integration (Trapezoidal and Simpson's rule), Simultaneous equations, Matrix addition and	20

	multiplication, Statistical analysis. QBASIC programs for Chemistry problems - Example: plotting van der Waals Isotherms (Simple Problem, available in general text books) and observe whether van der Waal gas equation is valid at temperatures lower than critical temperature where we require to solve a cubic equation and calculation of area under the curves (Complicated Problem, not available in general text books).	
3	**Use of Software Products** Computer Software like Scilab, Excel, LibreOffice and Calc , to solve some of the plotting or calculation problems, Handling of experimental data	08
	TOTAL	48

Suggested Readings :

1. McQuarrie, D. A.(2008), Mathematics for Physical Chemistry, University Science Books.
2. Mortimer, R.(2005), Mathematics for Physical Chemistry,3rd Edition, Elsevier.
3. Steiner, E.(1996),The Chemical Maths Book, Oxford University Press.
4. Yates, P. (2007),Chemical Calculations, CRC Press.
5. Harris, D. C.(2007),Quantitative Chemical Analysis,6th Edition, Freeman, Chapters 3-5.

DSE3 : Computer programs using QBASIC based on numerical methods (Practical: 2 credits)

Practical :

1. Roots of equations: (e.g. volume of gas using van der Waals equation and comparison with ideal gas, pH of a weak acid).
2. Numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).
3. Numerical integration (e.g. entropy/ enthalpy change from heat capacity data).
4. Probability distributions (gas kinetic theory) and mean values.
5. Mean, standard deviation and Least square curve fitting method for linear equation.
6. Matrix operations: addition, multiplication and transpose
7. Graphic programs related to Chemistry problems. e.g. van der Waals isotherm, Compressibility versus pressure curves, Maxwell distribution curves, concentration-time graph, pH metric titration curve, conductometric titration curves, Lambert Beer's law graph, s, p, d orbital shapes, radial distribution curves, particle in one dimensional box.

Use of Software Products

2. Computer Software like Scilab and Excel, etc for data handling and manipulation.
3. Simple exercises using molecular visualization software.
4. Open source chemistry software to draw structures.

Practical:

1. Levie, R.D.(2001),How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge University Press.
2. Noggle, J. H.(1985), Physical Chemistry on a Microcomputer, Little Brown & Co.
3. Venit, S.M.(1996),Programming in BASIC: Problem solving with structure and style, Jaico Publishing House.

DSE4 : Analytical Methods in Chemistry

Course Outcomes

After the completion of the course, the student will be able to:

CO1: Perform experiment with accuracy and precision.
CO2: Develop methods of analysis for different samples independently.
CO3: Test contaminated water samples.

CO4: Understand basic principle of instrument like Flame Photometer, UV-vis spectrophotometer.
CO5: Learn separation of analytes by chromatography.
CO6: Apply knowledge of geometrical isomers and keto-enol tautomers to analysis.
CO7: Determine composition of soil.
CO8: Estimate macronutrients using Flame photometry.

DSE4 : Analytical Methods in Chemistry (Theory:4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Qualitative and quantitative aspects of analysis:** Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression. Normal law of distribution of indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals.	08
2	**Optical methods of analysis** Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules UV-Visible Spectrometry: Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument; Transmittance. Absorbance and Beer-Lambert law Basic principles of quantitative analysis: estimation of metal ions from aqueous solution, geometrical isomers, keto-enol tautomers. Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs). Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal, Techniques for the quantitative estimation of trace level of metal ions from water samples.	15
3	**Thermal methods of analysis:** Theory of thermogravimetry (TG) and basic principle of instrumentation of thermal analyser. Techniques for quantitative estimation of Ca and Mg from their mixture.	07
4	**Electroanalytical methods** Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations.Techniques used for the determination of equivalence points. Techniques used for the determination of pKa values.	08
5	**Separation techniques** Solvent extraction: Classification, principle and efficiency of the technique. Mechanism of extraction: extraction by solvation and chelation, Technique of extraction: batch, continuous and counter current extractions, Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and non- aqueous media. Chromatography: Classification, principle and efficiency of the technique, Mechanism of separation: adsorption, partition & ion-exchange, Development of chromatograms: frontal, elution and displacement methods.	10
	TOTAL	48

Suggested Readings :

1. Willard, H.H.(1988),Instrumental Methods of Analysis, 7th Edition, Wardsworth Publishing Company.

2. Christian, G.D.(2004),Analytical Chemistry, 6th Edition, John Wiley & Sons, New York.
3. Harris, D. C.(2007),Quantitative Chemical Analysis,6th Edition, Freeman.
4. Khopkar, S.M. (2008), Basic Concepts of Analytical Chemistry, New Age International Publisher.
5. Skoog, D.A.; Holler F.J.; Nieman, T.A. (2005), Principles of Instrumental Analysis, Thomson Asia Pvt. Ltd.

DSE4 : Analytical Methods in Chemistry (Practical: 2 credits)
Practical : 1. Separation of mixtures by paper chromatography and reporting the Rf values: (i) Co^{2+} and Ni^{2+}. (ii) Amino acids present in the given mixture. 2. Solvent Extractions (i) To separate a mixture of Ni^{2+} & Fe^{2+} by complexation with DMG and extracting the Ni^{2+} DMG complex in chloroform, and determine its concentration by spectrophotometry. 3. Analysis of soil: (i) Determination of pH of soil. (ii) Total soluble salt (iii) Estimation of calcium and magnesium (iv) Qualitative detection of nitrate and phosphate 4. Ion exchange: (i) Determination of exchange capacity of cation exchange resins and anion exchange resins. (ii) Separation of amino acids from organic acids by ion exchange chromatography. 5. Spectrophotometry (i) Verification of Lambert-Beer's law and determination of concentration of a coloured species (CuSO4, KMnO4, CoCl2, CoSO4) (ii) Determination of concentration of coloured species via following methods; Graphical method, (b) Epsilon method, (c) Ratio method, (iv) Standard addition method

Practical:

1. Jeffery, G.H.; Bassett, J.; Mendham, J.; Denney, R.C.(1989),Vogel's Textbook of Quantitative Chemical Analysis,John Wiley and Sons.

DSE5 : Molecular Modelling and Drug Design

Course Outcomes

After the completion of the course, the student will be able to:

CO1: Understand theoretical background of computational techniques and selective application to various molecular systems.

CO2: Learn Energy minimization methods through use of different force fields.

CO3: Learn ESP Plots by suitable soft wares, electron rich and electron deficient sites,

CO4: Compare computational and experimental results and explain deviations.

CO5: Carry out Molecular dynamics (MD) and Monte Carlo (MC) simulations on several molecules and polymers.

CO6: Learn QSAR properties and their role in molecular modelling, cheminformatics and drug discovery.

CO7: Perform Optimization of geometry parameters of a molecule (such as shape, bond length and bond angle) through use of software like Chem Sketch and Argus Lab in interesting hands-on exercises.

DSE5 : Molecular Modelling and Drug Design (Theory:4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Introduction** Overview of Classical and Quantum Mechanical Methods (Ab initio, Semi-empirical, Molecular Mechanics, Molecular Dynamics and Monte Carlo) General considerations.	08

	Coordinate systems: Cartesian and Internal Coordinates, Bond lengths, bond angles and torsion angles, Writing Z -matrix (ex: methane, ethane, ethene, ethyne, water, H2O2	
2	**Potential Energy Surfaces** Intrinsic Reaction Coordinates, Stationary points, Equilibrium points – Local and Global minima, concept of transition state with examples: Ethane, propane, butane, cyclohexane. Meaning of rigid and relaxed PES. Applications of computational chemistry to determine reaction mechanisms. Energy Minimization and Transition State Search: Geometry optimization, Methods of energy minimization: Multivariate Grid Search, Steepest Descent Method, Newton-Raphson method and Hessian matrix.	08
3	**Molecular Mechanics:** Force Fields, Non-bonded interactions (van der Waals and electrostatic), how to handle torsions of flexible molecules, van der Waals interactions using Lennard-Jones potential, hydrogen bonding interactions, electrostatic term, Parameterization. Applications of MM, disadvantages, Software, Different variants of MM: MM1, MM2, MM3, MM4, MM+, AMBER, BIO+, OPLS.GUI.	08
4	**Molecular Dynamics:** Radial distribution functions for solids, liquids and gases, intermolecular Potentials (Hard sphere, finite square well and Lennard-Jones potential), concept of periodic box, ensembles (microcanonical, canonical, isothermal – isobaric), Ergodic hypothesis. Integration of Newton's equations (Leapfrog and Verlet Algorithms), Rescaling, Simulation of Pure water – Radial distribution curves and interpretation, TIP & TIP3P, Typical MD simulation Brief introduction to Langevin and Brownian dynamics Monte Carlo Method: Metropolis algorithm.	08
5	**HMO theory, Ab-initio methods & DFT** Huckel MO with examples: ethane, propenyl, cyclopropenyl systems, Properties calculated – energy, charges, dipole moments, bond order, electronic energies, resonance energies, Oxidation and reduction (cationic and anionic species of above systems) Extension to Extended Huckel theory and PPP methods Ab-initio methods: Writing the Hamiltonian of a system, Brief recap of H – atom solution, Units in quantum mechanical calculations, Born-Oppenheimer approximation (recap), Antisymmetry principle, Slater determinants, Coulomb and Exchange integrals, Examples of He atom and hydrogen molecule, Hartree-Fock method Basis sets, Basis functions, STOs and GTOs, diffuse and polarization functions. Minimal basis sets Advantages of ab initio calculations, Koopman's theorem, Brief idea of Density Functional Theory	08
6	**Semi-empirical methods and QSAR** Semi-empirical methods: Brief idea of CNDO, INDO, MINDO/3, MNDO, AM1, PM3 methods. Other file formats – PDB. Visualization of orbitals – HOMO, LUMO, ESP maps. QSAR: Structure-activity relationships. Properties in QSAR (Partial atomic charges, polarizabilities, volume and surface area, log P, lipophilicity and Hammet equation and applications, hydration energies, refractivity). Biological activities (LD50, IC50, ED50.)	08

	TOTAL	48

Suggested Readings :

1. Lewars, E. (2003), Computational Chemistry, Kluwer academic Publisher.
2. Cramer, C.J.(2004),Essentials of Computational Chemistry, John Wiley & Sons.
3. Hinchcliffe, A. (1996),Modelling Molecular Structures, John Wiley & Sons.
4. Leach, A.R.(2001),Molecular Modelling, Prentice-Hall.

DSE5 : Molecular Modelling and Drug Design
(Practical: 2 credits)

Practical :

1. Plotting a 3D graph depicting a saddle point in a spreadsheet software.
2. Determine the enthalpy of isomerization of cis and trans 2-butene.
3. Determine the heat of hydrogenation of ethylene.
4. Compare the optimized C-C bond lengths and Wiberg bond orders in ethane, ethene, ethyne and benzene using PM3. Is there any relationship between the bond lengths and bond orders? Visualize the highest occupied and lowest unoccupied molecular orbitals of ethane, ethene, ethyne, benzene and pyridine.
5. Perform a conformational analysis of butane.
6. Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine by comparison of their Mulliken charges and ESP maps.
7. Compare the gas phase basicities of the methylamines by comparing the enthalpies of the following reactions:

$BH^+ + NH3 \rightarrow B + NH4^+$

where B = CH3NH2, (CH3)2NH, (CH3)3N

8. Arrange 1-hexene, 2-methyl-2-pentene, (E)-3-methyl-2-pentene, (Z)-3-methyl-2-pentene, and 2,3- dimethyl-2-butene in order of increasing stability.
9. Compare the optimized bond angles H2O, H2S, H2Se using PM3.
10. Compare the HAH bond angles for the second row hydrides (BeH2, CH4, NH3, H2O) and compare with the results from qualitative MO theory.
11. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2- propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 ºC, 100 ºC, 108 ºC, 82 ºC, respectively).
12. Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
13. Plot the electrostatic potential mapped on electron density for benzene and use it to predict the type of stacking in the crystal structure of benzene dimer.
14. Predict the aromaticity of thiophene with respect to benzene by comparing the enthalpies of the following reactions:
    (a) Hydrogenation of benzene to 1,3-cyclohexadiene and then 1,3-cyclohexadiene to cyclohexene. (b)
15. Docking of Sulfonamide-type D-Glu inhibitor into MurD active site using Argus lab.

Note: Software: Argus Lab (www.planaria-software.com).

Practical:

1. Lewars, E. G. (2011),Computational Chemistry, Springer (India) Pvt. Ltd. Chapter 1 & 2.
2. Engel, T.; Reid, P.(2012),Physical Chemistry, Prentice-Hall. Chapter 26.

DSE6 : Polymer Chemistry

Course Outcomes

After the completion of the course, the student will be able to:

- **CO1:** Know about history of polymeric materials and their classification
- **CO2:** Learn about different mechanisms of polymerization and polymerization techniques
- **CO3:** Evaluate kinetic chain length of polymers based on their mechanism
- **CO4:** Differentiate between polymers and copolymers
- **CO5:** Learn about different methods of finding out average molecular weight of polymers
- **CO6:** Differentiate between glass transition temperature (Tg) and crystalline melting point (Tm)
- **CO7:** Determine Tg and Tm
- **CO8:** Know about solid and solution properties of polymers
- **CO9:** Learn properties and applications of various useful polymers in our daily life.

DSE6 : Polymer Chemistry (Theory:4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Introduction and history of polymeric materials** History of polymeric materials, Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of Polymers Functionality and its importance: Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization Bifunctional systems, Poly-functional systems	10
2	**Kinetics of Polymerization** Mechanism of step growth polymerization, kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic), Mechanism and kinetics of copolymerization, polymerization techniques	10
3	**Crystallography and polymers** Glass transition temperature (Tg) and determination of Tg, Free volume theory, WLF equation, Factors affecting glass transition temperature (Tg). Crystallization and crystallinity: Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point. Nature and structure of polymers-Structure Property relationships	10
4	**Molecular weight calculation, solubility and degradation characteristics of polymers** Determination of Molecular weight of polymers ((Mn, Mw, etc.) by end group analysis, viscometry, light scattering and osmotic pressure methods. Molecular weight distribution and its significance. Polydispersity index Polymer Solution Criteria for polymer solubility and Solubility parameter, Thermodynamics of polymer solutions, entropy, enthalpy and free energy change of mixing of polymers solutions. Polymer Degradation	09

	Thermal, oxidative, hydrolytic and photodegradation	
5	**Properties of Polymers** (Physical, thermal, Flow & Mechanical Properties) Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride) and related polymers, poly(vinyl acetate) and related polymers, acrylic polymers, fluoro polymers, polyamides and related polymers. Phenol formaldehyde resins (Bakelite, Novolac), polyurethanes, silicone polymers, polydienes, Polycarbonates, Conducting Polymers: polyacetylene, polyaniline, poly(p-phenylene sulphide, polypyrrole, polythiophene	09
	TOTAL	48

Suggested Readings :

1. Carraher,C. E. Jr. (2013), Seymour's Polymer Chemistry, Marcel Dekker, Inc.
2. Odian, G. (2004), Principles of Polymerization, John Wiley.
3. Billmeyer, F.W. (1984),Text Book of Polymer Science, John Wiley.
4. Ghosh, P. (2001),Polymer Science & Technology, Tata Mcgraw-Hill.
5. Lenz, R.W. (1967),Organic Chemistry of Synthetic High Polymers, Intersecience (Wiley).

DSE6 : Polymer chemistry
(Practical: 2 credits)

Practical :

Polymer synthesis

1. Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA)/Methyl Acrylate (MA).
2. Preparation of nylon 6,6
3. Redox polymerization of acrylamide
4. Precipitation polymerization of acrylonitrile
5. Preparation of urea-formaldehyde resin
6. Preparations of novalac resin/resold resin.
7. Microscale Emulsion Polymerization of Poly(methylacrylate).

Polymer characterization

1. Determination of molecular weight of polyvinyl propylidene in water by viscometry:
2. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of head-to-head monomer linkages in the polymer.
3. Determination of molecular weight by end group analysis of polymethacrylic acid.

Polymer analysis

1. Estimation of the amount of HCHO in the given solution by sodium sulphite method
2. IR studies of polymers
3. DSC (Differential Scanning Calorimetry) analysis of polymers
4. TG-DTA (Thermo-Gravimetery-Differential Thermal Analaysis) of polymers

Suggested Additional Experiment:

1. Purification of monomer.
2. Emulsion polymerization of a monomer.

Practical:

1. Allcock, H.R.; ; Lampe, F. W.; Mark, J. E.(2003),Contemporary Polymer Chemistry, Prentice Hall.
2. Fried, J.R. (2003), Polymer Science and Technology, Prentice-Hall.
3. Munk, P.; Aminabhavi, T. M. (2002), Introduction to Macromolecular Science, John Wiley & Sons.
4. Sperling, L.H.(2005),Introduction to Physical Polymer Science, John Wiley & Sons.

DSE7 : Research Methodology For Chemistry

Course Outcomes

After the completion of the course, the student will be able to:

- **CO1:** Learn how to identify research problems.
- **CO2:** Evaluate local resources and need for addressing the research problem
- **CO3:** Find out local solution.
- **CO4:** Know how to communicate the research findings.

DSE7 : Research Methodology For Chemistry (Theory:4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Literature Survey** Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples. Digital: Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups and communities, Blogs, Preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki- Databases, ChemSpider, Science Direct, SciFinder, Scopus. Information Technology and Library Resources: The Internet and World Wide Web. Internet resources for chemistry. Finding and citing published information. Open source Lead lectures. Open source chemistry designing sources, Essentials of Problem formulation and communication with society.	15
2	**Methods of Scientific Research and Writing Scientific Papers** Reporting practical and project work. Idea about public funding agencies of research, Writing literature surveys and reviews. Organizing a poster display. Giving an oral presentation. Writing scientific papers – justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work. Writing ethics. Avoiding plagiarism. Assessment of locally available resources.	10
3	**Chemical Safety and Ethical Handling of Chemicals** Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation. Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric level. Safe storage and disposal of waste chemicals. Recovery, recycling and reuse of laboratory chemicals. Procedure for laboratory disposal of explosives. Identification, verification and segregation of laboratory waste.Disposal of chemicals in the sanitary sewer system.Incineration and transportation of hazardous chemicals.	10
4	**Data Analysis** The Investigative Approach: Making and Recording Measurements. SI Units and their use. Scientific method and design of experiments. Analysis and Presentation of Data: Descriptive statistics. Choosing and using statistical tests. Chemometrics. Analysis of variance (ANOVA),	08

	Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial fitting, linearizing transformations, exponential function fit, r and its abuse. Basic aspects of multiple linear regression analysis. Biostatistics: brief introduction and data handling.	
5	**Exposure of chemistry software** Chemistry Students must be given exposure to applications of molecular modelling softwares e.g. Hyperchem, Schrodinger etc. Hands on experiments of docking.	05
	TOTAL	48

Suggested Readings :

1. Dean, J.R.; Jones, A.M.; Holmes, D;, Reed, R.; Jones, A.Weyers, J. (2011),Practical skills in chemistry, Prentice-Hall.
2. Hibbert, D.B.; Gooding, J.J. (2006),Data analysis for chemistry, Oxford University Press.
3. Topping, J.(1984),Errors of observation and their treatment, Chapman Hall, London
4. Levie, R. de.(2001),How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge University Press.
5. Le, C.T.; Eberly,L.E. (2016),Introductory Biostatistics, Wiley.

Additional Resources:

1. Chemical safety matters IUPAC – IPCS, Cambridge University Press, 1992.
2. OSU safety manual 1.01.

DSE8 : Green Chemistry

Course Outcomes

After the completion of the course, the student will be able to:

CO1: Understand the twelve principles of green chemistry and will build the basic understanding of toxicity,hazard and risk of chemical substances.

CO2: Understand stoichiometric calculations and relate them to green chemistry metrics.They will learn about atom economy and how it is different from percentage yield.

CO3: Learn to design safer chemical ,products and processes that are less toxic,than current alternatives. Hence,they will understand the meaning of inherently safer design for accident prevention and the principle "what you don't have can't harm you"

CO4: Understand benefits of use of catalyst and bio catalyst ,use of renewable feed stock which helps in energy efficiency and protection of the environment, renewable energy sources, importance led reactions in various green solvents.

CO5: Appreciate the use of green chemistry in problem solving skills, critical thinking and valuable skills to innovate and find out solution to environmental problems. Thus the students are able to realise that chemistry can be used to solve rather than cause environmental problems.

CO6: Green chemistry is a way to boost profits, increase productivity and ensure sustainability with absolute zero waste. Success stories and real world cases also motivate them to practice green chemistry.These days customers are demanding to know about a product: Is it green? Does it contribute to global warming? Was it made from non depletable resources? Students have many career opportunities as " green" is the path to success.

DSE8 : Green Chemistry (Theory:4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Introduction to Green Chemistry** What is Green Chemistry? Some important environmental laws, pollution prevention Act of 1990, emergence of green chemistry, Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry	05

2	Twelve principles of Green Chemistry and their explanation with examples Special emphasis on the following: Prevention of Waste/ by products; maximum incorporation of the materials used in the process into the final products , Environmental impact factor, waste or pollution prevention hierarchy Green metrics to assess greenness of a reaction, e.g. Atom Economy, calculation of atom economy of the rearrangement, addition, substitution and elimination reactions. Prevention/ minimization of hazardous/ toxic products reducing toxicity Risk = (function) hazard x exposure Designing safer chemicals with minimum toxicity yet has the ability to perform the desired functions Green solvents: super critical fluids with special reference to carbon dioxide, water as a solvent for organic reactions, ionic liquids, fluorous biphasic solvent, PEG, solventless processes, solvents obtained from renewable resources and how to compare greenness of solvents Energy requirements for reactions – alternative sources of energy: use of microwaves , ultrasonic energy and photochemical energy Selection of starting materials; should be renewable rather than depleting, Illustrate with few examples such as biodiesel and polymers from renewable resources (such as green plastic) Avoidance of unnecessary derivatization – careful use of blocking/protecting groups Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; catalysis and green chemistry, comparison of heterogeneous and homogeneous catalysis, biocatalysis, asymmetric catalysis and photocatalysis. Design for degradation: A product should not persist after the commercial function is over e.g. soaps and detergents, pesticides and polymers Strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes. Prevention of chemical accidents designing greener processes, inherent safer design, principle of ISD "What you don't have cannot harm you", greener alternative to Bhopal Gas Tragedy (safer route to carcarbaryl) and Flixiborough accident (safer route to cyclohexanol) subdivision of ISD, minimization, simplification, substitution, moderation and limitation.	15
3	**Examples of Green Synthesis/ Reactions** Green Synthesis of the following compounds: adipic acid, catechol, disodium iminodiacetate (alternative to Strecker synthesis). Green Reagents: Non-phosgene Isocyanate Synthesis, Selective Methylation using dimethylcarbonate. Microwave assisted solvent free synthesis of copper phthalocyanine Microwave assisted reactions in water: Hofmann Elimination, methyl benzoate to benzoic acid and Decarboxylation reaction Ultrasound assisted reactions: sonochemical Simmons-Smith Reaction (Ultrasonic alternative to Iodine)	10
4	**Real world case studies based on the Presidential green chemistry awards of EPA** Surfactants for Carbon Dioxide – replacing smog producing and ozone depleting solvents with CO2 for precision cleaning and dry cleaning of garments. A new generation of environmentally advanced wood preservatives: Getting the chromium and Arsenic out of pressure treated wood. An efficient, green synthesis of a compostable and widely applicable plastic (polylactic acid) made from corn. Healthier Fats and oils by Green Chemistry: Enzymatic Inter esterification for production of No Trans-Fats and Oils. Development of Fully Recyclable Carpet: Cradle to Cradle Carpeting.	09
5	**Future Trends in Green Chemistry**	09

	Oxidation reagents and catalysts; Biomimcry and green chemistry, Biomimetic, Multifunctional Reagents; mechanochemical and solvent free synthesis of inorganic complexes; co crystal controlled solid state synthesis (C^2S^3); Green chemistry in sustainable development.	
	TOTAL	48

Reading List :

Theory:

1. Anastas, P.T.; Warner, J.C.(1998),Green Chemistry, Theory and Practice, Oxford University Press.
2. Lancaster, M.(2016),Green Chemistry An Introductory Text.2nd Edition, RSC Publishing.
3. Cann , M. C. ;Connely,M. E.(2000), Real-World cases in Green Chemistry, American Chemical Society, Washington.
4. Matlack, A.S.(2001),Introduction to Green Chemistry, Marcel Dekker.
5. Alhuwalia,V. K.; Kidwai, M.R.(2005),New Trends in Green chemistry, Anamalaya Publishers.

Additional References:

1. Cann , M. C.; Umile, T.P. (2008), Real world cases in Green chemistry Vol 11, American chemical Society,Washington.
2. Benyus,J. (1997),Innovations Inspired by nature,Harper collins.
3. Garay,A. L; Pichon, A.; James,S.L. Chem Soc Rev, 2007, 36,846-855.

DSE8 : Green chemistry
(Practical: 2 credits)

Practical :

Characterization by m. pt., U.V.-Visible spectroscopy, IR spectroscopy, and any other specific method should be done (wherever applicable).

Safer starting materials

1.Preparation and characterization of nanoparticles of gold using tea leaves/silver nanoparticles using plant extracts.

Using renewable resources

2. Preparation of biodiesel from waste cooking oiland characterization (TLC, pH, Solubility, Combustion Test, Density, Viscosity, Gel Formation at Low Temperature and IR can be provided).

Use of enzymes as catalysts

3. Benzoin condensation using Thiamine Hydrochloride as a catalyst instead of cyanide.

Alternative green solvents

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

5. Mechanochemical solvent free, solid–solid synthesis of azomethine using p- toluidine and o-vanillin/p- vanillin (various other combinations of primary amine and aldehyde can also be tried).

Alternative sources of energy

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

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

Reducing waste

8. Designing and conducting an experiment by utilizing the products and by products obtained in above preparations which become waste otherwise if not used. This is done by critical thinking and literature survey.

Some representative examples:

- Use of nanoparticles as catalyst for a reaction
- Benzoin converted into Benzil and Benzil into Benzilic acid by a green method
- Use of azomethine for complex formation
- Rearrangement reaction from Benzopinacol to Benzopinacolone
- Conversion of byproduct of biodiesel to a useful product
- Students should be taught to do spot tests for qualitative inorganic analysis for cations and anions, and qualitative organic analysis for preliminary test and functional group analysis.

Practical:

1. Kirchoff, M.; Ryan, M.A. (2002), Greener approaches to undergraduate chemistry experiment. American Chemical Society, Washington DC.
2. Sharma, R.K.; Sidhwani, I.T.; Chaudhari, M.K.(2013), Green Chemistry Experiments: A monograph, I.K. International Publishing House Pvt Ltd. New Delhi.
3. Pavia,D.L.; Lamponam, G.H.; Kriz, G.S.W. B.(2006),Introduction to organic Laboratory Technique- A Microscale approach,4th Edition, Brrooks-Cole Laboratory Series for Organic chemistry.
4. Wealth from Waste: A green method to produce biodiesel from waste cooking oil and generation of useful products from waste further generated. Indu Tucker Sidhwani et al. University of Delhi, Journal of Undergraduate Research and Innovation, Volume 1, Issue 1,February 2015, ISSN: 2395-2334.
5. Sidhwani, Tucker I.; Chowdhury, S. Greener alternatives to Qualitative Analysis for Cations without H2S and other sulfur containing compounds, J. Chem. Educ. 2008, 85, 1099.
6. Sidhwani, Tucker I.; Chowdhury, S. et al., DU Journal of Undergraduate Research and Innovation, 2016, Volume 2, Issue 2, 70-79.
7. Dhingra, S., ;Angrish, C. Qualitative organic analysis: An efficient, safer, and economical approach to preliminary tests and functional group analysis. Journal of Chemical Education, 2011, 88(5), 649-651.

DSE9 : Industrial Chemicals and Environment

Course Outcomes

After the completion of the course, the student will be able to:

CO1: The different toxic gases and their toxicity hazards
CO2: Safe design systems for large scale production of industrial gases.
CO3: Manufacturing processes, handling and storage of inorganic chemicals.
CO4: Hazardous effects of the inorganic chemicals on human beings and vegetation.
CO5: The requirement of ultra-pure metals for the semiconducting technologies
CO6: Composition of air, various air pollutants, effects and control measures of air pollutants.
CO7: Different sources of water, water quality parameters, impacts of water pollution, water treatment.
CO8: Different industrial effluents and their treatment methods.
CO9: Different sources of energy.
CO10: Generation of nuclear waste and its disposal.
CO11: Use of biocatalyst in chemical industries.

DSE9 : Industrial Chemicals and Environment (Theory:4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Industrial Gases:** Large scale production, uses storage and hazards in handling of the following gases: oxygen, nitrogen, argon, neon, helium, hydrogen, acetylene, carbon monoxide, chlorine, fluorine, and sulphur dioxide.	05
2	**Inorganic Chemicals:** Manufacture, applications, analysis and hazards in handling the following chemicals: hydrochloric acid, nitric acid, sulphuric acid, caustic soda, borax, bleaching powder, sodium thiosulphate, hydrogen peroxide, potassium dichromate and potassium permanganate	08

3	**Industrial Metallurgy:** Preparation of ultrapure metals for semiconductor technology.	05
4	**Environment and its segments:** Ecosystems. Biogeochemical cycles of carbon, nitrogen and sulphur. Air Pollution: Major regions of atmosphere,chemical and photochemical reactions in atmosphere. Air pollutants: types, sources, particle size and chemical nature; Photochemical smog: its constituents and photochemistry. Major sources of air pollution, Pollution by SO2, CO2, CO, NOx, H2S and other foul smelling gases, methods of estimation of CO, NOx, SOx and control procedures, Effects of air pollution on living organisms and vegetation Greenhouse effect and Global warming, Environmental effects of ozone, Ozone depletion by oxides of nitrogen, chlorofluorocarbons and halogens, Air pollution control, Settling Chambers, Venturi Scrubbers, Cyclones, Electrostatic Precipitators (ESPs).	15
5	**Water Pollution:** Hydrological cycle, water resources, aquatic ecosystems, Sources and nature of water pollutants, Techniques for measuring water pollution, Impacts of water pollution on hydrological cycle and ecosystems. Water purification methods. Effluent treatment plants (primary, secondary and tertiary treatment). Industrial effluents from the following industries and their treatment: electroplating, textile, tannery, dairy, petroleum and petrochemicals, agro fertilizer. Sludge disposal. Industrial waste management, incineration of waste. Water treatment and purification (reverse osmosis, electro dialysis, ion exchange). Water quality parameters for wastewater, industrial water and domestic water.	08
6	**Energy & Environment:** Sources of energy: Coal, petrol and natural gas. Nuclear fusion / fission, solar, hydrogen, geothermal, tidal and hydel. Nuclear Pollution: Disposal of nuclear waste, nuclear disaster and its management. Biocatalysis: Introduction to biocatalysis: Importance in green chemistry and chemical industry.	07
	TOTAL	48

Suggested Readings :

1. Manahan, S.E. (2017),Environmental Chemistry, CRC Press
2. Buchel, K.H.; Moretto, H.H.; Woditsch, P.(2003),Industrial Inorganic Chemistry, Wiley-VCH.
3. De, A.K.(2012), Environmental Chemistry, New Age International Pvt., Ltd.
4. Khopkar, S.M.(2010), Environmental Pollution Analysis, New Age International Publisher.

DSE9 : Industrial Chemicals and Environment (Practical: 2 credits)
Practical : **Industrial Chemicals & Environment** 1. Determination of dissolved oxygen in water.

2. Determination of Chemical Oxygen Demand (COD).
3. Determination of Biological Oxygen Demand (BOD).
4. Percentage of available chlorine in bleaching powder.
5. Measurement of chloride, sulphate and salinity of water samples by simple titration method (AgNO3 and potassium chromate).
6. Estimation of total alkalinity of water samples (CO32-, HCO3-) using double titration method.
7. Measurement of dissolved CO2
8. Determination of hexavalent Chromium Cr(VI) concentration in tannery wastes/waste water sample using UV-Vis spectrophotometry technique.
9. Preparation of borax/ boric acid

Practical :

1. Vowles, P.D.; Connell, D.W. (1980),Experiments in Environmental Chemistry: A Laboratory Manual, Vol.4, Pergamon Series in Environmental Science.
2. Gopalan, R.; Anand, A.; Sugumar R.W. (2008),A Laboratory Manual for Environmental Chemistry, I. K. International.

DSE10 : Instrumental Methods of Chemical Analysis

Course Outcomes

After the completion of the course, the student will be able to:

CO1: Handle analytical data
CO2: Understand basic components of IR, FTIR, UV-Visible and Mass spectrometer.
CO3: Interpret of IR, FTIR, UV-visible spectra and their applications.
CO4: Understand the use of single and double beam instruments.
CO5: Learn separations techniques like Chromatography.
CO6: Learn elemental analysis, NMR spectroscopy, Electroanalytical Methods, Radiochemical Methods, X-ray analysis and electron spectroscopy.

DSE10 : Instrumental Methods of Chemical Analysis (Theory:4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	**Introduction to analytical methods of data analysis** Treatment of analytical data, including error analysis. Classification of analytical methods and the types of instrumental methods. Consideration of electromagnetic radiations.	08
2	**Molecular spectroscopy** Infrared spectroscopy: Interaction of radiations with molecules: absorption and scattering. Means of excitation (light sources), separation of spectrum (wavelength dispersion, time resolution), detection of the signal (heat, differential detection), interpretation of spectrum (qualitative, mixtures, resolution), advantages of Fourier-Transform Infrared (FTIR) spectroscopy. Applications: Issues of quality assurance and quality control, special problems for portable instrumentation and rapid detection.	08
3	**UV-Visible/ Near IR Spectroscopy** Emission, absorption, fluorescence and photoacoustic. Excitation sources (lasers, time resolution), wavelength dispersion (gratings, prisms, interference filters, laser, placement of sample relative to dispersion, resolution), Detection of signal (photocells, photomultipliers, diode arrays, sensitivity and S/N), Single and double beam instruments, Interpretation (quantification, mixtures, absorption vs. fluorescence and the use of time, photoacoustic, fluorescent tags).	08
4	**Separation techniques**	08

	Chromatography: Gas chromatography, liquid chromatography, Importance of column technology (packing, capillaries), Separation based on increasing number of factors (volatility, solubility, interactions with stationary phase, size, electrical field), Detection: simple vs. specific (gas and liquid), Detection as a means of further analysis (use of tags and coupling to IR and MS), Electrophoresis (plates and capillary) and use with DNA analysis. Immunoassays and DNA techniques.	
5	**Mass spectroscopy** Making the gaseous molecule into an ion (electron impact, chemical ionization), Making liquids and solids into ions (electrospray, electrical discharge, laser desorption, fast atom bombardment), Separation of ions on basis of mass to charge ratio, Magnetic, Time of flight, Electric quadrupole. Resolution, time and multiple separations, detection and interpretation.	08
6	**Elemental analysis** Mass spectrometry (electrical discharges). Atomic spectroscopy: Atomic absorption, atomic emission, and atomic fluorescence. Excitation and getting sample into gas phase (flames, electrical discharges, plasmas), wavelength separation and resolution (dependence on technique), detection of radiation (simultaneous/scanning, signal noise), interpretation (errors due to molecular and ionic species, matrix effects, other interferences). NMR spectroscopy: Principle, Instrumentation, Factors affecting chemical shift, Spin-coupling, Applications. Electroanalytical Methods: Potentiometry & Voltammetry.(Lectures: 4) Radiochemical Methods.(Lectures: 4) X-ray analysis and electron spectroscopy (surface analysis).(Lectures: 4)	08
	TOTAL	48

Suggested Readings :

1. Willard, H.H.; Merritt, L.L. Jr.; Dean, J.A.; Settle, F.A. Jr.(2004), Instrumental methods of analysis, 7th edition, CBS Publishers.
2. Christian, G.D.(2004),Analytical Chemistry, 6th Edition, John Wiley & Sons, New York.
3. Skoog, D.A.; Holler, F. J.; Crouch, S.(2006),Principles of Instrumental Analysis,Thomson Brooks/Cole.
4. Banwell, C.N. (2006),Fundamentals of Molecular Spectroscopy,Tata McGraw-Hill Education

DSE10 : Instrumental Methods of Chemical Analysis
(Practical: 2 credits)

Practical :

Instrumental methods of chemical analysis

1. Determination of the isoelectric pH of a protein.
2. Titration curve of an amino acid.
3. Determination of the void volume of a gel filtration column.
4. Determination of a mixture of cobalt and nickel (UV-visible spectroscopy).
5. Study of electronic transitions in organic molecules (i.e., acetone in water).
6. IR absorption spectra (study of aldehydes and ketones).
7. Determination of calcium, iron, and copper in food by atomic absorption spectroscopy.
8. Quantitative analysis of mixtures by gas chromatography (i.e., chloroform and carbon tetrachloride).
9. Separation of carbohydrates by HPLC.
10. Determination of caffeine in beverages by HPLC.
11. Potentiometric titration of a chloride-iodide mixture.

12. Cyclic voltammetry of the ferrocyanide/ferricyanide couple.
13. Use of nuclear magnetic resonance instrument and to analyse the spectra of methanol and ethanol
14. Use of fluorescence to do "presumptive tests" to identify blood or other body fluids.
15. Use of "presumptive tests" for anthrax or cocaine.
16. Collection, preservation, and control of blood evidence being used for DNA testing.
17. Use of capillary electrophoresis with laser fluorescence detection for nuclear DNA (Y chromosome only or multiple chromosome).
18. Use of sequencing for the analysis of mitochondrial DNA.
19. Laboratory analysis to confirm anthrax or cocaine.
20. Detection in the field and confirmation in the laboratory of flammable accelerants or explosives.
21. Detection of illegal drugs or steroids in athletes.
22. Detection of pollutants or illegal dumping.
23. Fibre analysis.

Practical:

1. Skoog, D. A.; Holler, F. J.; Crouch, S.(2006),Principles of Instrumental Analysis, Cengage Learning.

GENERIC ELECTIVE

GE1 : Atomic Structure, Bonding, General Organic Chemistry and Aliphatic hydrocarbons

COURSE OUTCOMES:

After of end of this course the students of other course will get idea about :
CO1 : fundamentals of atomic structure and bondig.
CO2 : concepts of basic organic chemistry and aliphatic hydrocarbons.

DSE10 : Instrumental Methods of Chemical Analysis (Theory:4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	Atomic structure : Bohr's theory, its limitations and hydrogen spectrum,,de Broglie equation, Heisenberg's Uncertainty principle , Quantum numbers and its significance, shapes of s,p,d and f orbitals , Pauli exclusion principle,Hund's rule of maximun spin multiplicity .	12
2	Bonding : Ionic bond and its general characteristics, type of ions ,ionic size ,radius ratio,packing of ions in crysttal ,Covalent bond,Lewis structure ,Valence bond theory of covent bonding , Hybridization VSPER theory,shapes of simple covent molecules, concepts of sigma and pi bonding , bond length and bond angles , Molecular orbital theory, moleclar orbital diagram of homo-nulear diatomic molecules , MO diagram of CO and NO.Fujan's rule, , Metallic bond , conductivity of metals , Vander wall's force and its applications , Hydrogen bond and its applications.	12
3	General Orgaic Chemistry : Nomenclature of branced alkanes and nomenclature of poly- functional group containing compounds, effect of hybridisation on the shape and bond strength in organic molecules , Electron displacement effects : inductive effect , electromeric effect, resonance/mesomeric effect ,hyper-conjugative effect applications of electron displacement effects , Electrophilic and nucleophilic reagents , fission of bonds :hetrolysis and homolysis , shapes and relative stability of carbocations, , carbanions , free radicals , carbenes. Type of organic reactions : addition , substitution and elimination reactions.	12
4	Aliphatic hydrocarbons: Preparation of alkanes ,conversions of functional	12

	group containing compounds into alkane. Wolf Kishner's reductin , Clemensons reduction, Wurtz reaction, selectivity in halogenation of alkanes , Preparation of alkenes and alkynes ,E1 , E2 and E1CB reactions , Saytzeff's and Hofmann's eliminations, common electrophilic additions eg hydrohalogenation, halogenation , Glyoxylation, Ozonolysis ,Hydroboration-oxidation , acidity of alkynes and alkylation of alkynes.	
TOTAL		48

Suggested Readings :

1. Organic Chemistry by Morrison and Boyd
2. Inorganic Chemisry published by S.Chand& company.

GE1 : Atomic Structure, Bonding, General Organic Chemistry and Aliphatic hydrocarbons

The studends are directed to perform the following practicals :-

CO1 : Crystallization of impure organic compounds by using cold or hot water , water -ethanol mixture , ethanol .

CO2 : Determination of boiling point of supplied organic liquid .

GE1 : Atomic Structure, Bonding, General Organic Chemistry and Aliphatic hydrocarbons (Practical: 2 credits)
Practical : 1. Determination of melting points of supplied organic solids. 2. Detection of nitrogen in given organic compound . 3. Tests of unsaturation in supplied organic compounds . 4. Nitration of benzene and phenol. 5. Benzolyation of Phenol.

Practical:

1. Practical Organic Chemistry : N.K .Vishnoi.
2. Practical Organic Chemistry: S.Cand &company.

GE2 : Chemical Energetics, Equilibria and functional group 1 containing organic compounds

COURSE OUTCOMES:

After the end of this course the students of other course will get basic idea about

CO1 : Chemical energetics and various type of equilibria

CO2: the reactions of alkyl halides and alcohols.

GE2 : Chemical Energetics, Equilibria and functional group 1 containing organic compounds (Theory:4 credits)		
Unit	**Topics to be covered**	**No. of Lectures**
1	Chemical energetics : Intrinsic energy , concept of enthalpy ,Enthalpy of reactions , enthalpy of formation, enthalpy of combustion, enthalpy of neutralization, enthalpy of solution ,Hess's law of constant heat summation ,Reversible and irreversible process, Isothermal process, Adiabatic process, isochric and isobaric process , cyclic process , First law of thermodynamics ,work done in isothermal reversible process , work dobe in adiabatic reversible process , concept of Entropy and Gibbs free energy , spantaneous process , second law of thermodynamics.	12

2	Equilibria : Reversible and irreversible chemical reactions , Chemical equilibrium , Law of mass action , Equilibrium constant- Kc, Kp and Kx with their inter relationship, calcutions related of equilibrium constants , Ionic Equilibrium, pH of solutions , pH scale , Buffer solutions : acidic and basic buffers , Handerson's equation for the calculation of the pH of buffer solutions , common ion effect , solubility product and its significance. Concepts of hydrolysis of salt.	12
3	Function group :1 containg organic compounds : Halogen derivatives Preparation of alkyl halides , nucleophilic substitution in alkyl halides, leaving ability of the functional groups , SN2 and SN1 reactions , role of solvent .	12
4	Functional group 1 containing organic compounds : Alcohols Preparation of alcohols, solubility of different type of alchols , relative boiling points ,dehydration of alcohols, reactions related with alcohols.	12
TOTAL		**48**

Suggested Readings :

1. Text book of Physical Chemistry : Puri,Sharma and Pathania.
2. Organic Chemistry : B.S.Bahl and Arun Bahl

GE2 : Chemical Energetics, Equilibria and functional group 1 containing organic compounds (Practical) (Practical: 2 credits)
Practical : 1.Determination of water equivalent of calorimeter. 2.Determination of heat of neutralization by using strong acid and strong base. 3.Calculation of pH change of a solution due to the addition of HCl or NaOH. 4.Preparation of acidic buffer solution and its pH change calcutions. 5.Preparation of basic buffer solution and its pH change calculations.

Practical:

1. Practical Physical Chemistry : Bharti Bhawan Prakashan.