

# **Central University of Punjab, Bathinda**



## **Course Structure and Syllabus**

**M.Sc. Chemistry**

**Session: 2020-22**

**Department of Chemistry**

**School of Basic and Applied Sciences**

**Program Outcomes**

Upon successful completion of the course work, student will be able to

- equip with state of art of knowledge of different areas of chemistry
- develop the employability skills required for chemical industry and pharmaceutical companies

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## SEMESTER I

S. No.	Course Code	Course Title	Course Type	L	T	P	Cr
1	CHM.509	Inorganic Chemistry-1	CC	3	0	0	3
2	CHM.510	Organic Chemistry-I	CC	4	0	0	4
3	CHM.511	Physical Chemistry-I	CC	3	0	0	3
4	CHM.512	Quantum Chemistry	CC	3	0	0	3
5	CHM.513	Practical Inorganic Chemistry-I	SB	0	0	4	2
6	CHM.514	Practical Organic Chemistry-I	SB	0	0	4	2
7	CHM.506	Fundamental Biology (Non-medical group)	CF	2	0	0	2
8	CHM.507	Fundamental Mathematics (Medical group)					
<b>Opt any one of the following Elective/MOOC courses:</b>							
9	CHM.508	Analytical Chemistry and Instrumental Methods	EC	4	0	0	4
10	CHM.577	Environmental Chemistry					
11	CHM.520	Green Chemistry					
12	CHM.541	Seminar	SB	0	0	0	1
13	XXX	Inter-Disciplinary Course (Opt any one from other Departments)	ID	2	0	0	2
<b>Total</b>				<b>21</b>	<b>0</b>	<b>8</b>	<b>26</b>
<b>Inter-Disciplinary Course for other Departments</b>							
14	CHM.515	Basics perspective in Inorganic Chemistry	ID	2	0	0	2
15	CHM.516	Introduction to Green Chemistry and Sustainability	ID	2	0	0	2
16	CHM.519	Chemicals of Everyday Life	ID	2	0	0	2

**CC:** Core Course, **EC:** Elective Course, **CF:** Compulsory Foundation, **EF:** Elective Foundation, **SB:** Skill Based

**L: Lectures T: Tutorial P: Practical Cr: Credits**

**Criteria for evaluation of theory exams:** Internal 75% (Quiz – 10%, Assignment and Term Paper – 15%, MST – 25%, EST I- 25%); EST II- 25%.

**Criteria for evaluation of Seminar and Practical exams:** Continuous Assessment= 50% Marks, End term = 50%.

## SEMESTER II

S. No.	Course Code	Course Title	Course Type	L	T	P	Cr
1	CHM.521	Inorganic Chemistry-II	CC	4	0	0	4
2	CHM.522	Organic Chemistry-II	CC	4	0	0	4
3	CHM.523	Physical Chemistry-II	CC	3	0	0	3
4	CHM.526	Practical Inorganic Chemistry-II	SB	0	0	4	2
5	CHM.527	Practical Physical Chemistry- II	SB	0	0	4	2
<b>Opt any Two of the following courses:</b>							
6	CHM.524	Spectroscopic Analysis	EC	4	0	0	4
7	CHM.525	Molecular Spectroscopy		4	0	0	4
8	CHM.578	Inorganic Photochemistry		4	0	0	4
9	CHM.542	Seminar	SB	0	0	0	1
10	XXX	Inter-Disciplinary Course (Opt any one from other Departments)	ID	2	0	0	2
<b>Total</b>				<b>21</b>	<b>0</b>	<b>8</b>	<b>26</b>
<b>Inter-Disciplinary Course for other Departments</b>							
11	CHM.517	Chemistry of Nanomaterials and Fabrication	ID	2	0	0	2
12	CHM.518	General Laboratory Practices	ID	2	0	0	2

**CC:** Core Course, **EC:** Elective Course, **CF:** Compulsory Foundation, **EF:** Elective Foundation, **SB:** Skill Based

**L: Lectures T: Tutorial P: Practical Cr: Credits**

**Criteria for evaluation of theory exams:** Internal 75% (Quiz – 10%, Assignment and Term Paper – 15%, MST – 25%, EST I- 25%); EST II- 25%.

**Criteria for evaluation of Seminar and Practical exams:** Continuous Assessment= 50% Marks, End term = 50%.

### SEMESTER III

S. No.	Course Code	Course Title	Course Type	L	T	P	Cr
1.	CHM.551	Inorganic Chemistry-III	CC	4	0	0	4
2.	CHM.552	Organic Chemistry-III	CC	4	0	0	4
3.	CHM.554	Practical Organic Chemistry-III	SB	0	0	4	2
4.	CHM.555	Practical Physical Chemistry- III	SB	0	0	4	2
5.	CHM.556	Research Methodology	CF	2	0	0	2
<b>Opt any one of the following courses:</b>							
6.	CHM.553	Bioinorganic and Biophysical Chemistry	EC	3	0	0	3
	CHM.571	Polymer and Solid State Chemistry		3	0	0	3
	CHM.579	Current Trends in Organic Synthesis		3	0	0	3
7.	CHM.558	Protein Chemistry	VAC	1	0	0	1
8.	CHM.599	Project	SB	0	0	0	6
	<b>Total</b>			<b>14</b>	<b>0</b>	<b>8</b>	<b>24</b>

**CC:** Core Course, **EC:** Elective Course, **CF:** Compulsory Foundation, **EF:** Elective Foundation, **SB:** Skill Based

**L: Lectures T: Tutorial P: Practical Cr: Credits**

**Criteria for evaluation of theory exams:** Internal 75% (Quiz – 10%, Assignment and Term Paper – 15%, MST – 25%, EST I- 25%); EST II- 25%.

**Criteria for evaluation of Seminar and Practical exams:** Continuous Assessment= 50% Marks, End term = 50%.

### SEMESTER IV

S. No.	Course Code	Course Title	Course Type	L	T	P	Cr
1.	CHM.572	Concepts in Chemistry –I	DEC	2	0	0	2
2.	CHM.573	Concepts in Chemistry –II	DEC	2	0	0	2
3.	CHM.599	Project	SB	0	0	0	6
<b>Opt any two of the following courses:</b>							
4.	CHM.574	Advanced Organic Synthesis	EC	4+4	0	0	4+4
	CHM.575	Chemistry of Natural Products					
	CHM.576	Organotransition Metal Chemistry					
	CHM.580	Supramolecular Chemistry					
	CHM.581	Material Chemistry					
5.	CHM.557	Basic Instrumentation and Sensors	VAC	1	0	0	1
6.	CHM.598	Seminar	SB	0	0	0	1
		<b>Total</b>		<b>13</b>	<b>0</b>	<b>0</b>	<b>20</b>

**Criteria for evaluation of theory exams:** Internal 75% (Quiz – 10%, Assignment and Term Paper – 15%, MST – 25%, EST I- 25%); EST II- 25%.

**Criteria for evaluation of Seminar and Practical exams:** Continuous Assessment= 50% Marks, End term = 50%.

## SEMESTER I

**Course Title: Fundamental Biology (Non-medical group)**

**Course Code: CHM.506**

**Total Contact Hours: 30**

L	T	P	Cr
2	0	0	2

**Learning Outcome:** After this course completion, students will be able to

- Molecular structure and interactions present in proteins, nucleic acids, carbohydrates and lipids.
- Organization and working principles of various components present in living cell.
- Physical principles of structure, function, and folding of biomolecules.

### Unit I

**7 Hours**

**Introduction:** Cell structure and functions, thermodynamics and kinetics of biological processes, ATP. Interactions in aqueous solutions, Role of water in life, pH, Acidic and basic buffers, Biological buffers, solution equilibria, Henderson-Hasselbalch equation, Hofmeister series, Chaotropic and kosmotropic ions/co-solvents.

### Unit II

**7 Hours**

**Amino Acids and Peptides:** Classification and properties of amino acids, peptide and polypeptides, primary structures, structure of peptide bond, synthesis of peptides, different protecting groups in peptide chemistry, N-terminal, C-terminal and sequence determination.

**Carbohydrates:** Biologically important monosaccharides, disaccharides and polysaccharides, glycoproteins, role of sugars in biological recognition.

### Unit III

**8 Hours**

**Proteins:** Secondary structure of proteins with emphasize on supramolecular characteristics of  $\alpha$ -helix,  $\beta$ -, supersecondary structure and triple helix structure of collagen, tertiary structure of protein-folding, quaternary structure of protein, in-vivo and in-vitro protein folding, protein misfolding and conformational diseases.

### Unit IV

**8 Hours**

**Nucleic Acids:** Purine and pyrimidine bases, nucleotides, nucleosides, base pairing via H-bonding, structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA, different types of RNA and their functions, the chemical basis for heredity, overview of replication of DNA, transcription, translation and genetic code.

**Lipids:** Lipid classification, lipid bilayers, lipoproteins-composition. high density (HDL) and low-density (LDL) lipoproteins and function, membrane proteins - integral membrane proteins.

**Mode of Transactions:** Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brain storming, Tutorial

**Suggested Readings**

1. Voet, D., Voet, J. G., and Pratt, C. W. (2008). *Principle of Biochemistry*. John Wiley and Sons .
2. Berg, J. M., Stryer, L., and Tymoczko, J. L. (2015). *Stryer Biochemie*. Springer-Verlag.
3. Garrett, R. H., and Grisham, C. M. (2013). *Biochemistry*, Brooks/Cole, Cengage Learning.
4. Conn, E., and Stumpf, P. (2009). *Outlines of Biochemistry*. John Wiley and Sons.

L	T	P	Cr
2	0	0	2

**Course Title: Fundamental Mathematics (Medical group)**

**Course Code: CHM.507**

**Total Contact Hours: 30**

**Learning Outcome:** The students will be able to

- Demonstrate and apply the various mathematical operations including matrix operations, differentiation, integration, complex, quadratic and differential equations for common problems in chemistry.

**Unit I**

**7 Hours**

**Trigonometry and Algebra**

**Trigonometric functions:** Trigonometric operations for sum and differences of angles, addition and subtraction formulas.

**Algebra:** Polynomial equations and their solutions: binomial theorem and expansion. Common series and expansions used in chemistry.

**Complex Algebra:** Complex numbers, the graphical interpretation of complex numbers, characterizations of the exponential function, the trigonometric functions of complex argument ( $e^{i\theta}$ ,  $e^{-i\theta}$ ).

**Unit II**

**8 Hours**

**Differential Calculus**

Functions, limits, continuity, first principle of differentiation, basic rules of differentiation, maxima and minima, exact and inexact differentials, partial differentiation, application to solution of potential energy, van der waals radii, velocity and Boltzmann distribution.

**Matrix Algebra:** Addition and multiplication; inverse, adjoint and transpose of matrices, matrix equation, Introduction to vector spaces, matrix Eigen values and Eigen vectors, diagonalization, determinants (examples from Huckel theory).

**Unit III**

**8 Hours**

**Integral Calculus**



Basic rules for integration, integration by parts, partial fraction and substitution, definite integrals, evaluation of definite and some standard integrals related to chemistry

#### **Unit IV**

**7 Hours**

**Elementary Differential Equations:** Variables-separable and exact, first-order differential equations, homogenous, exact and linear equations. Applications to chemical kinetics, quantum chemistry, etc. solutions of differential equations by the power series method, spherical harmonics, second order differential equations and their solutions.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

#### **Suggested Readings**

1. Steiner, E. (2008). *The Chemistry Maths Book*. Oxford University Press.
2. Doggett, G., and Sutcliffe, B. T. (1995). *Mathematics for Chemistry*. Longman Pub Group.
3. Daniels, F. (2003). *Mathematical Preparation for Physical Chemistry*. McGraw Hill Publishers.
4. Tebbutt, P. (1998). *Basic Mathematics for Chemists*. Chichester: Wiley.

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
4	0	0	4

**Course Title: Analytical Chemistry and Instrumental Methods**

**Course Code: CHM.508**

**Total Contact Hours: 45**

**Learning Outcome:** The students will be able to

Determine method of analysis based on the sample amount/volume, accuracy and precision required for analysis and interference.

Know the application of the principles of instrumental analysis.

#### **Unit I**

**15 Hours**

**Quantitative Analysis:** Concepts important to quantitative analysis, classification of methods for quantitative analysis, choice of method for analysis, theory of volumetric method of analysis, acid-base, redox, argentometric/precipitation and complexometric titrations methods of analysis with examples including functional group analysis, alkalinity, hardness, COD/BOD etc.

**Gravimetric Analysis:** Nucleation, supersaturation, peptization, co-crystallization, mixed crystal formation, occlusion, filtration, drying and use of thermogravimetry for Gravimetric analysis.

#### **Unit 2**

**15 Hours**

**Analytical Spectroscopy:** Principle, applications and limitations of spectrophotometry, Beer-Lambert law, Single and double beam UV-Visible Spectrometer, principle of detectors, sources and treatment of interferences,

spectrum and absorbance mode analysis with emphasis on mixtures analysis, and detection limits of method, isosbestic point and its physical significance, method of continuous variation for evaluation of stability constant calculation and Job's Plot method for stoichiometry of complexes, and fluorescence spectrometry and Benesi-Hilderbrand method for 1:1 stoichiometry complexes.

Atomic Absorption spectroscopy: General principle behind atomic spectroscopy, flame photometry and its instrumentation, atomic absorption spectrometry (AAS); flame AAS, electrothermal AAS (ETAAS).Hollow Cathode lamp, Deuterium, Smith-Hieftje and Zeeman background corrections.Sample preparation and analysis, blank and standard runs, chemical and physical interferences and its removal using ionization suppressors, matrix modifiers and protective agents.Introduction to ICP and ICP-MS techniques of analysis.

### **Unit III**

**15 Hours**

**Potentiometry:** General principles, reference electrodes, ion selective electrodes, ion selective electrode construction, membrane electrode, glass membrane electrodes, liquid membrane electrodes, Eu-doped-lanthanum fluoride electrode, biosensors.

**Coulometry:** Basic principles of electrogravimetry, ohmic potential, kinetic and concentration polarization, overpotential, constant current and constant potential coulometry. coulometric titrations and application e.g. Redox titration and Karl-Fischer Titration for moisture analysis.

**Voltammetry:** Principles, dropping mercury electrode (DME), polarography, half-wave potential, diffusion current and Ilkovic equation, different wave forms—linear scan, square scan and triangular scan.polarography, cyclic, differential pulse andAnion/cation stripping voltametryand their applications.

### **Unit IV**

**15 Hours**

**Chromatography:** Partition and distribution, principles of chromatography, plate and rate theory. retention time and retention factor, resolution and separation factor; general idea about adsorption, partition and column chromatography, paper and thin layer chromatography, gas chromatography (GC) and high performance liquid chromatography (HPLC) - instrumentation, methodology and applications. SFC LC, hyphenated techniques. Ion exchange resins and extraction, Ion Chromatography, anion suppressors and ion speciation analysis.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

### **Suggested Readings**

1. Skoog, D. A., Holler, F. J., and Crouch, S. R. (2017). *Principles of Instrumental Analysis*. Cengage learning.
2. Willard, H. H., Merritt Jr, L. L., Dean, J. A., and Settle Jr, F. A. (1988). *Instrumental Methods of Analysis*.CBS Publishers.

- Mendham, J., Denney, R. C., Barnes, J. D., and Thomas, M. J. K. (2008). *Vogel's Textbook of Quantitative Chemical Analysis*, Dorling Kindersley.
- Skoog, D. A., West, D. M., Holler, F. J., and Crouch, S. (2013). *Fundamentals of Analytical Chemistry*. Nelson Education.
- Christian, G. D. (1994). *Analytical Chemistry*. John Wiley and Sons, USA, 331.
- Bard, A. J., and Faulkner, L. R. (2001). *Electrochemical Methods*, 2nd. John Wiley New York, 669.
- Rouessac, F., and Rouessac, A. (2013). *Chemical Analysis: Modern Instrumentation Methods and Techniques*. John Wiley and Sons.
- Danzer, K. (2007). *Analytical Chemistry: Theoretical and Metrological Fundamentals*. Springer Science and Business Media.

L	T	P	Cr
3	0	0	3

**Course Title: Inorganic Chemistry - I**

**Course Code: CHM.509**

**Total Contact Hours: 45**

**Learning Outcome:** The completion of this course the student's will able learn

- Reaction mechanism, formation constant and stability of the coordination complexes.
- Interpretation of the electronic properties.
- Interpretation of the magnetic properties

### **Unit I**

**11 Hours**

**Metal-Ligand Equilibria in Solution:** Stepwise and overall formation constant and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by spectrophotometry and potentiometric (pH) methods.

### **Unit II**

**11 Hours**

**Reaction Mechanisms of Transition Metal Complexes:** Introduction, potential energy diagram and reactivity of metal complexes, ligand substitution reactions, labile and inert metal complexes, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, anation reaction, substitution reactions in square planar complexes, trans effect, mechanism of the substitution reaction reactions without metal ligand bond cleavage, electron transfer processes outer and inner sphere.

### **Unit III**

**12 Hours**

Ligand field theory and molecular orbital theory; nephelauxetic series, structural distortion and lowering of symmetry, electronic, steric and Jahn-Teller effects on energy levels, conformation of chelate ring, structural equilibrium, magnetic properties of transition metal ions and free ions presentive, effects of L-S

coupling on magnetic properties, quenching of orbital angular momentum by crystal fields in complexes in terms of splitting. effect of spin-orbit coupling and A, E and T states mixing.

#### Unit IV

11 Hours

**Crystal Fields Splitting:** Spin-spin, orbital-orbital and spin orbital coupling, LS and J-J coupling schemes, determination of all the spectroscopic terms of  $p^n$ ,  $d^n$  ions, determination of the ground state terms for  $p^n$ ,  $d^n$ ,  $f^n$  ions using L.S. scheme, determination of total degeneracy of terms, order of interelectronic repulsions and crystal field strength in various fields, spin orbit coupling parameters ( $\lambda$ ) energy separation between different j states, the effect of octahedral and tetrahedral fields on S, P, D and F terms. Splitting patterns of and G, H and I terms. selection rules of electronic transitions in transition metal complexes, relaxation of the selection rule in centrosymmetric and non-centrosymmetric molecules, Orgel diagrams, Tanabe Sugano diagrams, spectrochemical series, band intensities, factors influencing band widths.

**Mode of Transactions:** Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brain storming, Tutorial

#### Suggested Readings

1. Cotton, F. A., and Wilkinson, G. (1988). *Advanced Inorganic Chemistry* (Vol. 545). New York: Wiley.
2. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic Chemistry: Principles of Structure and Reactivity*. Pearson Education India.
3. Greenwood, N. N., and Earnshaw, A. (2012). *Chemistry of the Elements*. Elsevier.
4. Miessler, G. L. and Tarr, D. A. (2011) *Inorganic Chemistry*, Pearson Education.
5. Atkins, P. (2010). *Shriver and Atkins' Inorganic Chemistry*. Oxford University Press, USA.
6. Dutta, R. L., and Syamal, A. (1993). *Elements of Magnetochemistry*. Affiliated East-West Press.
7. Drago, R. S. (1992) *Physical Methods for Chemists*. Saunders College Publishing.

**Course Title: Organic Chemistry-I**

**Course Code: CHM.510**

**Total Contact Hours: 60**

L	T	P	Cr
4	0	0	4

**Learning Outcome:** After the completion of the course students will be able to

- Identify various methods and intermediate species involved while determining the mechanism of organic reactions.
- Examine the mechanistic and synthetic aspects of nucleophilic and electrophilic substitution reactions.

- Explore the implication of enolate chemistry for the synthesis of various molecules.

### Unit I

15 Hours

**Reaction mechanism, structure and reactivity:** Classification and determination of reaction mechanisms, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, methods of determining mechanisms, isotope effects, effect of structure on reactivity: Hammett equation, Taft equation.

**Reactive intermediates:** Generation, structure and reactions of carbocations, carbanions, free radicals, carbenes, nitrenes and benzyne. Neighbouring group participation, classical and non-classical carbocations, phenonium ions and norbornyl system.

**Aromaticity:** Aromaticity in benzenoid and non-benzenoid compounds, antiaromaticity, homoaromatic compounds.

### Unit II

15 Hours

**Aliphatic nucleophilic substitution reaction:** The  $S_N^2$ ,  $S_N^1$ , mixed  $S_N^2$  and  $S_N^1$ , the  $S_N^i$  mechanism. Energy profile diagram, nucleophilic substitution at an allylic, aliphatic and vinylic carbon. reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, regioselectivity, effect of solvent in substitution reaction, competition between  $S_N^2$  and  $S_N^1$  mechanisms.

**Aromatic nucleophilic substitution:** The  $S_N^{Ar}$ , bimolecular displacement mechanism and benzyne mechanism, reactivity effect of substrate structure, leaving group and attacking nucleophile.

**Aromatic electrophilic substitution:** The arenium ion mechanism, orientation and reactivity, energy profile diagrams, *ortho/para* ratio, *ipso* attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles.

### Unit III

15 Hours

**Elimination reactions:** E2, E1 and E1cB mechanisms and their spectrum, orientation of the double bond, effects of substrate structures, attacking base, the leaving group and the medium, mechanism and orientation in pyrolytic elimination.

**Addition to carbon-carbon multiple bonds:** Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, addition of halogen polar reagents to alkenes, Regio- and chemoselectivity, orientation and reactivity, hydroboration, epoxidation and hydroxylation.

### Unit IV

15 Hours

**Addition to carbon-hetero multiple bonds:** Structure and reactivity of carbonyl group towards nucleophilic addition: addition of CN, ROH, RSH, H<sub>2</sub>O, hydride ion, ammonia derivatives, LiAlH<sub>4</sub>, NaBH<sub>4</sub>, organozinc and organolithium

reagents to carbonyl and conjugated carbonyl compounds, Arndt-Eistert synthesis. Mechanism of condensation reactions involving enolates: Aldol, Knoevenagel, Claisen, Dieckmann, Mannich, Benzoin, Perkin and Stobber reactions. Carboxylic acids and derivatives, hydrolysis of esters and amides, ammonolysis of esters.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

### Suggested Readings

1. Clayden, J., Greeves, N., Warren, S. and Wothers, P. (2012) *Organic Chemistry*, Oxford University Press.
2. Finar, I. L. (1996). *Textbook Of Organic Chemistry*. ELBS, Pearson Education UK.
3. McMurry, J. (1996). *Organic Chemistry*, Brooks. Cole, New York, 657.
4. Smith, M. B., and March, J. (2013). *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*. John Wiley and Sons.
5. Ahluwalia, V. K., and Parashar, R. K. (2011). *Organic Reaction Mechanisms*. Narosa Publishing House (P) Ltd.
6. Bansal, R. K. (2012). *A Textbook of Organic Chemistry*. New Age International.
7. Bansal R.K. (2010) *Organic Reaction Mechanism*. New Age International (P) Ltd.
8. Kalsi, P.S. (2010) *Organic Reactions and Their Mechanisms*. New Age International, New Delhi.
9. Lowry, T. H. and Richardson K. S. (1998) *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., New York.
10. Morrison, R.T. and Boyd, R.N. (2011) *Organic Chemistry*, Prentice- Hall of India.
11. Mukherjee, S.M. and Singh, S.P. (2009) *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd., New Delhi.
12. Solomon, T.W.G, Fryhle, C.B. and Snyder, S. A. (2013) *Organic Chemistry*. John Wiley and Sons, Inc.
13. Sykes, P. A. (1997) *Guide Book to Mechanism in Organic Chemistry*, Prentice Hall.

**Course Title: Physical Chemistry-I**

**Course Code: CHM.511**

**Total Contact Hours: 45**

L	T	P	Cr
3	0	0	3

**Learning Outcome:** After the completion of the course students will be able to

- Interpret classical thermodynamics and thermodynamic phenomenon in a chemical system

- Explore the solutions of nonelectrolytes and electrolytes and draw the phase transition of different system
- Differentiate different statistical thermodynamics and thermodynamic properties in terms of partition functions,
- Explain Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, theories of specific heat for solids.

### **Unit I**

**11 Hours**

**Partial Molar Properties and Fugacity:** Partial molar properties. Chemical potential of a perfect gas, dependence of chemical potential on temperature and pressure, Gibbs- Duhem equation, fugacity, its importance and determination,

**Thermodynamics of Simple Mixtures:** Thermodynamic functions for mixing of perfect gases. Chemical potential of liquids. Raoult's law, thermodynamic functions for mixing of liquids (ideal solutions only). Real solutions and activities. Activity coefficient; determination of activity and activity coefficients.

### **Unit II**

**11 Hours**

**Solid-Liquid Solutions:** Solutions of nonelectrolytes and electrolytes. Colligative properties of solutions, such as osmotic pressure, depression of the freezing point and elevation of the boiling point.

**Phase transition:** Phase rule, water, CO<sub>2</sub> phase transition, binary and ternary component phase transitions. Clausius-Clapeyron equation and its application to solid-liquid, liquid-vapour and solid-vapour equilibria.

### **Unit III**

**12 Hours**

**Statistical Thermodynamics:** Statistical concepts and examples, Thermodynamic probability and entropy, Partition function, molar partition function, thermodynamic properties in term of molecular partition function for diatomic molecules, monoatomic gases, rotational, translational, vibrational and electronic partition functions for diatomic molecules, calculation of equilibrium constants in term of partition function.

### **Unit IV**

**11 Hours**

**Theories of Statistical Thermodynamics:** Concept of Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, Difference between Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, Applications of Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics., Monoatomic solids, theories of specific heat for solids.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

### Suggested Readings

1. Barrow, G. M. (2007) *Physical Chemistry*. Tata McGraw-Hill Publishers.
2. Kapoor, K. L. (2011) *Text Book of Physical Chemistry*. 3/5, Macmillan Publishers.
3. Atkins, P. and De Paula, J. (2009) *Atkins' Physical Chemistry*. Oxford University Press.
4. McQuarrie, D. A. and Simon, J. D. (1998) *Physical Chemistry: A Molecular Approach*. Viva Books.
5. Moore, J. W. and Pearson, R. G. (1981) *Kinetics and Mechanism*. John Wiley and Sons.
6. Silbey, R. J. Alberty, R. A. and Bawendi, M. G. (2004) *Physical Chemistry*. Wiley-Interscience Publication.
7. Engel, T., Reid, P. and Hehre, W. (2012) *Physical Chemistry*. Pearson Education.
8. Puri, B.R., Sharma L.R. and Pathania, M.S. (2013) *Principles of Physical Chemistry*. Vishal Publishing Company.
9. Rastogi, R. P. and Mishra, R. R. (2013) *An Introduction to Chemical Thermodynamics*. Vikas Publishing
10. Rajaram, J. and Kuriacose, J. C. (2013) *Chemical Thermodynamics, Classical, Statistical and Irreversible Thermodynamics*. Pearson Education.
11. Laurendeau N. M. (2005) *Statistical Thermodynamics: Fundamentals and Applications*. Cambridge University Press.
12. Nash, L. K. (2012) *Elements of Statistical Thermodynamics*. Dover Publication Inc.
13. Hill, T. L. (1986) *An Introduction to Statistical Thermodynamics*. Dover Publications Inc

**Course Title: Quantum Chemistry**

**Course Code: CHM.512**

**Total Contact Hours: 45**

L	T	P	Cr
3	0	0	3

**Learning Outcome:** The students will be able to

- Interpret and solve the Schrodinger equation various particle in a boundary model, Electronic and Hamiltonian operators for molecules.
- Explain the quantum chemical description of angular momentum and term symbols for a one and many-electron systems.
- Relate the Born-Oppenheimer approximation, the Pauli principle, Hund's rules, Hückel theory and the variation principle with the atomic and molecular phenomena.



**Unit I****11 Hrs**

**Fundamental Background:** Review of essential mathematical concepts required for quantum chemistry, Postulates of quantum mechanics, Eigen values and Eigen functions, operators, Schrodinger equation.

**Unit II****11 Hrs**

**Translational, Rotational and Vibrational Motions:** - Free particle and particle in a box and its application (*i.e.*, quantum tunnelling effect), one-dimensional harmonic oscillator and rigid rotor, particle in a ring, particle on a sphere, hydrogen like atoms

**Variation and Perturbation Methods:** The variation theorem and its application, linear variation principle, perturbation theory up to second order in energy and its applications.

**Unit III****12 Hrs**

**Angular Momentum:** Ordinary angular momentum, generalized angular momentum, Eigen functions and Eigen values for angular momentum, Ladder operator, addition of angular momenta, spin, antisymmetry and Pauli exclusion principle, Slaterdeterminantal wave functions.

**Electronic Structure of Atoms:** Electronic configuration, term symbols and spectroscopic states, Russell-Saunders terms and J-J coupling schemes, Term separation energies of pn and dn configurations, Magnetic effects: spin-orbit coupling and Zeeman splitting, Hartree-Fock (HF) or Self-consistent field (SCF) method.

**Unit IV****11 Hrs**

**Born-Oppenheimer Approximation:** LCAO-MO and VB treatments of the  $H_2^+$  and  $H_2$ , Shape of molecules, Hybridization and valence MOs of  $H_2O$  and  $NH_3$ . Determination of bond angle in  $sp^3$ ,  $sp^2$  and  $sp$ , Huckel Theory of acyclic and cyclic conjugated systems, Bond order and charge density calculations.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

**Suggested Readings**

1. Levine, I.N. (2000) *Quantum Chemistry*. Pearson Education Inc.
2. Chandra, A.K. (1994) *Introductory Quantum Chemistry*. Tata Mcgraw-Hill.
3. Prasad, R.K., (2009) *Quantum Chemistry*. New Age Science.
4. McQuarrie, D. A. and Simon, J. D. (1998) *Physical Chemistry: A Molecular Approach*. Viva Books.
5. Murrell, J.N., Kettle S.F.A. and Tedder, J. M. (1965) *Valence Theory*. John Wiley Publishers.
6. Lowe, J. P. and Peterson, K., (2006). *Quantum Chemistry*. Academic Press.

**Course Title: Practical Inorganic Chemistry-I**

**Course Code: CHM.513**

**Contact Hours: 60**

L	T	P	Cr
0	0	4	2

**Learning Outcome:** The students will be updated will able to

- Analyse of volumetric and gravimetric analysis of cations and anions within reaction mixtures.
- Standardization and titrations of various inorganic compounds.

**Experiments:**

**Introduction to good laboratory practices in chemistry.**

**Gravimetric Estimation**

1. Determination of  $\text{Ba}^{2+}$  as its sulphate/chromate.
2. Estimation of lead as its lead sulfate.
3. Estimation of Nickel (II) as its nickel dimethyl glyoximate.
4. Estimation of  $\text{Cu}^{2+}$  as cuprousthiocyanate.

**Precipitation Titrations**

1.  $\text{AgNO}_3$  standardization by Mohr's method.
2. Volhard's method for  $\text{Cl}^-$  determination.

**Oxidation-Reduction Titrations**

1. Standardization of  $\text{KMnO}_4$  with sodium oxalate and determination of  $\text{Ca}^{2+}$  ion.
2. Standardization of ceric sulphate with Mohr's salt and determination of  $\text{Cu}^{2+}$ ,  $\text{NO}_2$  and  $\text{C}_2\text{O}_4^{2-}$  ions.
3. Standardization of  $\text{K}_2\text{Cr}_2\text{O}_7$  with  $\text{Fe}^{2+}$  and determination of  $\text{Fe}^{3+}$  (Ferric alum)
4. Standardization of hypo solution with potassium iodate /  $\text{K}_2\text{Cr}_2\text{O}_7$  and determination of available  $\text{Cl}_2$  in bleaching powder,  $\text{Sb}^{3+}$  and  $\text{Cu}^{2+}$ .
5. Determination of hydrazine with  $\text{KIO}_3$  titration.

**Mode of Transactions:** Demonstration, PPT, videos, Lecture cum demonstration

**Suggested Readings**

1. Pass, G. and Sutcliffe H. (1979) *Practical Inorganic Chemistry*. Chapman and Hall Ltd.
2. Jolly, W.L. (1961) *Synthetic Inorganic Chemistry*. Prentice Hall, Inc.
3. Nakamoto, K. (1997) *Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A and B*. John Wiley and Sons, .
4. Mendham, J., Denney, R.C., Barnes, J.D. and Thomas, M. J. K. (2000) *Vogel's Textbook of Quantitative Chemical Analysis*, Pearson Education Ltd.
5. Svehla, G. and Sivasankar, B. (1996) *Vogel's Qualitative Inorganic Analysis*. Pearson Education Ltd.

6. Skoog, D.A., Holler, F.J. and Crouch, S.R.(2007) *Principles of Instrumental Analysis*. Thomson Learning.

**Course Title: Practical Organic Chemistry-I**

**Course Code: CHM.514**

**Total Contact Hours: 60**

L	T	P	Cr
0	0	4	2

**Learning Outcome:**At the end of this course student will be able to

- Exercise good laboratory practices including safe handling of hazardous chemicals, laboratory glassware and equipment(s).
- Apply various experimental skills for purification, isolation and recrystallization of organic molecules.
- Analyse the progress of a given reaction on thin layer chromatography.

**Experiments:**

**Safety and Handling of hazardous chemicals:**

- (i) Good laboratory practices, handling and disposal of hazardous chemicals.
- (ii) Awareness about different types of glassware, heating devices, equipment(s), how to conduct organic reaction etc.

**A. Techniques:**

**Chromatography:** Thin layer chromatography (TLC): Monitoring the progress of chemical reactions,  $R_f$  values: identification of unknown organic compounds by comparing the  $R_f$  values with known standards. Column chromatography.

**Purification Techniques:** crystallization, distillation, sublimation.

Determination of melting point and mixed melting point.

**B. Single Stage Synthesis:** Synthesis of compounds and their purification, aspects such as conversion, theoretical yield and percentage yield should be paid attention. (Attempt any six)

1. Synthesis of chalcones *via* Claisen-Schmidt condensation.
2. Reduction of benzophenone to benzhydral using  $\text{NaBH}_4$ .
3. Conversion of benzaldehyde to cinnamic acid (Knoevenagel condensation)
4. Conversion of benzaldehyde to dibenzylidene acetone (Aldol condensation)
5. To prepare phenylpropene *via* dehydration of corresponding phenylpropanol.
6. To prepare ethyl cinnamate *via* acid catalyzed esterification of cinnamic acid.
7. Conversion of phthalic anhydride to phthalimide
8. To synthesize acylinide analogue of Meldrum acid.
9. Synthesis of alcohol *via* addition of Grignard reagent to an aldehyde.

**C. ChemDraw-Sketch:** Draw the structure of simple aliphatic, aromatic, heterocyclic organic compounds with substituents. Get the correct IUPAC name.

**Mode of Transactions:** Demonstration, PPT, videos, Lecture cum demonstration

**Suggested Readings**

1. Harwood, L.M. and Moody, C.J. (1989) *Experimental Organic Chemistry*. Blackwell Scientific Publishers.
2. Vogel, A.I. (1978) *Textbook of Practical Organic Chemistry*. ELBS, Longman Group Ltd.
3. Mann, F.G. and Saunders, B.C. (1975) *Practical Organic Chemistry*. Orient Longman Pvt. Ltd.
4. Leonard, J. and Lygo, B. (1995) *Advanced Practical Organic Chemistry*. Chapman and Hall,.
5. Armarego, W.L. and Chai, C. (2012) *Purification of Laboratory Chemicals*. Butterworth-Heinemann.
6. Young, J.A. (1991) *Improving Safety in the Chemical Laboratory: A Practical Guide*. Wiley Publishing.

**Course Title: Green Chemistry**  
**Course Code: CHM.520**

L	T	P	Cr
4	0	0	4

**Learning outcome:** Students will be able to

- Differentiate various aspects of green chemistry for sustainable development
- Utilize ionic liquids and solid supported reaction conditions to reduce or eliminate use of volatile organic solvents
- Use water as solvent in chemical transformations
- Utilize energy efficient MW and sonicator in organic synthesis

**Unit I**

**15 Hours**

**Introduction to green chemistry:** History, need and goals. Green chemistry and sustainability, dimensions of sustainability, limitations/obstacles in pursuit of the goals of green chemistry. Opportunities for the next generation of materials designers to create a safer future. Basic principles of green chemistry: Atom economy and scope, Prevention/Minimization of hazardous/toxic products, Designing safer chemicals, Selection of appropriate auxiliary substances (solvents, separation agents etc), use of renewable starting materials, Avoidance of unnecessary derivatization-careful use of blocking/protection groups. Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents, Designing biodegradable products, Prevention of chemical accidents,

Strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes. Development of accurate and reliable sensors and monitors for real time in process monitoring.

## **Unit II**

**15 Hours**

**Green Solvents:** Role of solvents in chemical synthesis, Environmental and health concerns of organic solvents, Need for Alternative/Cleaner solvents, Criteria for selection and design of green solvents Water: the natural solvent on earth, organic reactions: hydrophobic effects enhancing the reaction selectivities, low solubility of O<sub>2</sub> in water, water soluble catalysts, challenges in using water as solvent,

**Ionic liquids:** physicochemical properties, Synthesis of Ionic Liquids, Directed Inorganic and Organometallic Synthesis, formation of oxides, electrochemical synthesis in ionic liquids,

**Glycerol:** solvent properties, volatility, polarity, availability, glycerol as a solvent combining the advantages of water and ionic liquids, enhancement of reaction selectivity, glycerol as a solvent for catalyst design and recycling, separation processes and material synthesis in glycerol, examples of synthesis of transition metal and metal oxide crystals

Supercritical fluids: supercritical CO<sub>2</sub> and its properties, advantages of using CO<sub>2</sub> as solvent, Synthesis of metal nanoparticles, CO<sub>2</sub> as solvent for coatings and lithography, biomaterial processing, other supercritical fluids.

## **Unit III**

**15 Hours**

**Microwave induced and ultrasound assisted green synthesis:** Introduction to synthetic organic transformation under microwave (i) Microwave assisted reactions in water (ii) Microwave assisted reactions in organic solvents. (iii) Microwave solvent free reactions Ultrasound assisted reactions: Introduction, substitution reactions, addition, oxidation, reduction reactions. Biocatalysts in organic synthesis: Introduction, Biochemical oxidation and reductions.

## **Unit IV**

**15 Hours**

**Approaches to green synthesis:** Use of green reagents: polymer supported reagents: peptide coupling reagents. Green catalysts, Phase-transfer catalysts in green synthesis. Advantages of PTC, Application of PTCs in C-alkylation, N-alkylation, S-alkylation. Darzens reaction, Williamsons synthesis, Wittig reaction, Click Chemistry. Use of Crown ethers in esterification, saponification, anhydride formation, aromatic substitution and elimination reactions.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

**Suggested Readings:**

1. Ahulwalia, V.K.; Kidwai M. (2004). *New Trends in Green Chemistry*, Springer
2. Anastas, P.T.; Warner J. C. (2000). *Green chemistry, Theory and Practical*. Oxford University Press.
3. Grieco, P.A. (1997). *Organic Synthesis in Water*. Publisher: Kluwer Academic.
4. Peter Wasserscheid and Tom Welton (2008), *Ionic Liquids in Synthesis*, WILEY-VCH Verlag GmbH & Co. KGaA, 2008.
5. Sheldon, R.A., Arends, I. and Hanefeld U. (2007), *Green Chemistry and Catalysis*, WILEY-VCH Verlag GmbH & Co. KGaA.
6. William M. N.; (2003) *Green Solvents for Chemistry: Perspectives and Practice*, Oxford University Press.

**Course Title: Seminar****Course Code: CHM.541****Total Contact Hours: 15**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Cr</b>
0	0	0	1

**Learning Outcome:** The student will be able to

- Elucidate and demonstrate the technical writing and present the problem in hand highlighting the various ways the problem is addressed in the literature.

The seminar must include discussion on topics such as awareness about weapons of mass destruction (chemical, biological, radiological, and nuclear weapons), disarmament, peaceful uses of chemistry, International Regulation of Biological and Chemical or Weapons of Mass Destruction.

## SEMESTER II

**Course Title: Inorganic Chemistry-II**

**Course Code: CHM.521**

**Total Contact Hours: 45**

L	T	P	Cr
4	0	0	4

**Learning Outcome:** The students will be able to

- Concepts to realize point group within chemical structure, character tables and projection operator techniques.
- Application of symmetry and group theory in spectroscopy.
- Structural properties of organometallic complexes and their uses.

### Unit I

**15 Hours**

**Symmetry:** Symmetry elements, symmetry operations and their matrix representation, group postulates and types, multiplication tables, point group determination.

### Unit II

**15 Hours**

**Group theory:** Determination of reducible and irreducible representations, character tables, construction of character tables for  $C_{2v}$ ,  $C_{3v}$ , use of symmetry in obtaining symmetry of orbitals in molecules.

### Unit III

**16 Hours**

**Metal Complexes:** Organic-transition metal chemistry, complexes with  $\pi$ -acceptor and  $\sigma$ -donor ligands, 18-electron and 16-electron rules, isolobal analogy, Synthesis and important reaction of metal carbonyls. Structure and bonding of metal carbonyls, metal nitrosyl, dinitrogen and dioxygen complexes, tertiary phosphine as ligand and vibrational spectra of metal carbonyls for bonding and structure elucidation.

### Unit IV

**14 Hours**

**Inorganic cages:** Metallocenes, metal cluster compounds, metal-metal bond, metal carbenes, carbonyl and non-carbonyl clusters, fluxional molecules, application of organometallic compounds as catalysts in organic synthesis. Cage compounds of boron: boron cage compounds, boranes, carboranes and metallocenecarboranes.

**Mode of Transactions:** Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brain storming, Tutorial

### Suggested Readings

1. Cotton, F. A., and Wilkinson, G. (1988). *Advanced inorganic chemistry* (Vol. 545). New York: Wiley.
2. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic chemistry: principles of structure and reactivity*. Pearson Education India.

- Greenwood, N. N., and Earnshaw, A. (2012). *Chemistry of the Elements*. Elsevier.
- Lever, A.B.P. (1984) *Inorganic Electronic Spectroscopy*. Elsevier Science Publishers B.V.
- Atkins, P. (2010). *Shriver and Atkins' inorganic chemistry*. Oxford University Press, USA.
- Dutta, R. L., and Syamal, A. (1993). *Elements of magnetochemistry*. Affiliated East-West Press.

**Course Title: Organic Chemistry-II**

**Course Code: CHM.522**

**Total Contact Hours: 60**

L	T	P	Cr
4	0	0	4

**Learning Outcome:**The students will be able to

- Interpret and predict the energetically favoured conformation of cyclic and acyclic compounds, chirality and reactivity.
- Differentiate between thermally and photochemically driven pericyclic reactions and explain about their stereochemical aspects.
- Explore various molecular rearrangements in organic synthesis for the conversion of different functional group.

### Unit I

**16 Hours**

**Stereochemistry:** Chirality, projection formulae, configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, diastereoselectivity, D/L, R/S, E/Z and cis/trans configurational notations, *threo* and *erythro* isomers, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, conformational analysis of acyclic compounds and cyclic compounds such as cyclopentane, cyclohexane, cyclohexanone derivatives, decalins, 1,2, 1,3-, 1,4-disubstituted cyclohexane derivatives and D-Glucose, effect of conformation on reactivity,

### Unit II

**14 Hours**

**Photochemistry:** Jablonski diagram, singlet and triplet states, photosensitization, quantum efficiency, photochemistry of carbonyl compounds, Norrish type-I and type-II cleavages, Photochemistry of alkenes and enones, Paterno-Buchi reaction, Photoreduction, Di  $\pi$  - methane rearrangement. Photochemistry of aromatic compounds, Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction, Singlet molecular oxygen reactions.



### Unit III

16 Hours

**Pericyclic chemistry:** Introduction, Phases, nodes and symmetry properties of molecular orbitals in ethylene, 1,3-butadiene, 1,3,5-hexatriene, allyl cation, allyl radical, pentadienyl cation and pentadienyl radical.

**Electrocyclic reactions:** Conrotation and disrotation,  $4n$  and  $4n+2$  systems. Woodward-Hoffmann rules. (i) Symmetry properties of HOMO of open chain partner (ii) Conservation of orbital symmetry and correlation diagrams.

**Cycloaddition reactions:** Suprafacial and antarafacial interactions.  $\pi^2 + \pi^2$  and  $\pi^4 + \pi^2$  cycloadditions and stereochemical aspects. Diels-Alder reaction. Woodward-Hoffmann Selection rules. Explanation for the mechanism by (i) Conservation of orbital symmetry and correlation diagrams (ii) FMO theory

**Sigmatropic reactions:** [1,j] and [i,j] shifts; suprafacial and antarafacial, selection rules for [1, j] shifts; Cope and Claisen rearrangements; explanation for the mechanism by (i) symmetry properties of HOMO (ii) Introduction to cheletropic reactions and the explanation of mechanism by FMO theory.

### Unit IV

14 Hours

**Rearrangements:** General mechanistic considerations-nature of migration, migratory aptitude, mechanistic study of the following rearrangements: Pinacol-pinacolone, Wagner-Meerwein, Benzil-Benzilic acid, Favorskii, Neber, Beckmann, Hofmann, Curtius, Lossen, Schmidt, Carroll, Claisen, Cope, Gabriel-Colman, Smiles and Sommelet-Hauser rearrangements.

**Selective Name Reactions:** Ene/Alder-ene reaction, Dakin reaction, Reformatsky, Robinson annulation, Michael addition, Hofmann-Löffler Fretag, Chichibabin reaction.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

### Suggested Readings

1. Clayden, J., Greeves, N., Warren, S. and Wothers, P. (2012). *Organic Chemistry*. Oxford University Press.
2. Bansal, R. K. (2012). *A Textbook of Organic Chemistry*. New Age International.
3. Carey, F. A., and Sundberg, R. J. (2007). *Advanced Organic Chemistry: Part A: Structure and Mechanisms*. Springer Science and Business Media.
4. Kalsi, P. S. (2010). *Stereochemistry Conformation and Mechanism*. New Age International.
5. Eliel, E. L., and Wilen, S. H. (2008). *Stereochemistry of Organic Compounds*. John Wiley and Sons.
6. Carey, F. A., and Sundberg, R. J. (2007). *Advanced Organic Chemistry: Part B*. Springer Science and Business Media.
7. Finar, I. L. (1996). *Textbook of Organic Chemistry*. ELBS, Pearson Education UK.
8. Katritzky, A. R., Ramsden, C. A., Joule, J. A., and Zhidankin, V. V. (2010). *Handbook of Heterocyclic Chemistry*. Elsevier.

9. Norman, R.O.C. and Coxon, J.M. (1998). *Principles of Organic Synthesis*. Blackie Academic and Professional.
10. Fleming, I. (2015). *Pericyclic Reactions*. Oxford University Press.
11. Singh, J. (2005). *Photochemistry and Pericyclic Reactions*. New Age International.
12. McMurry, J. (1996). *Organic Chemistry*, Brooks. Cole, New York, 657.

**Course Title: Physical Chemistry-II**

**Course Code: CHM.523**

**Total Contact Hours: 45**

L	T	P	Cr
3	0	0	3

**Learning Outcome:** The students will be able to

- Evaluate and predict the spontaneity of a redox processes in electrochemical systems
- Apply activity coefficient calculated from Debye-Huckel theory in real chemical solutions.
- Establish and evaluate the kinetics and mechanism for catalytic and photo reactions, homogenous and heterogeneous catalysis reactions.
- Explore application different adsorption isotherms.
- Become expertises in various techniques for fast reaction monitoring.

### **Unit I**

**12 Hrs**

**Electrochemistry:** Ionic equilibria, electrolytic conductance –Kohlrausch's Law, activity-coefficients, mean activity coefficients; Debye-Huckel treatment of dilute electrolyte solutions, derivation of Debye-Huckel limiting law, extended Debye-Huckel law and conductometric titrations.

**Electrochemical Cells:** Nernst equation, redox systems, electrochemical cells, application of electrochemical cell, concentration cells with and without liquid junction, thermodynamics of reversible electrodes and reversible cells, potentiometric titration.

### **Unit II**

**11 Hrs**

**Reaction Kinetics:** Introduction, rates of chemical reactions, complex reactions, steady state approximation, determination of mechanisms of chemical reactions, temperature dependence of rate constant, Arrhenius and Eyring equations and their applications, collision and transition state theories of rate constant, Kramers theory of reaction kinetics, treatment of unimolecular reactions, steric factor, ionic reactions: salt effect,.

### **Unit III**

**11 Hrs**

**Photochemical Reactions and Processes:** Laws of photochemistry and kinetics of photochemical reactions, measurement of fluorescence and phosphorescence lifetimes and photoinduced electron transfer rates, photosensitization, quenching and photodimerization.

**Fast Reaction Kinetics:** Introduction to time-resolved techniques for absorption and emission measurements, relaxation method, study of kinetics of fast reactions by millisecond stopped-flow, nanosecond flash photolysis techniques, detection and kinetics of reactive intermediates,

#### **Unit IV**

**11 Hrs**

**Adsorption and Catalysis:** Adsorption of solids, Gibbs adsorption isotherm, BET adsorption isotherm, Langmuir and Fredulich Isotherms. Homogeneous catalysis and heterogeneous catalysis, enzyme catalysis. Michealis-Menten mechanism, Lineweaver-Burk Plot, competitive, non-competitive and uncompetitive bindings, kinetics of catalytic reactions.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

#### **Suggested Readings**

1. Laidler, K. J. (1987). *Chemical Kinetics*. Pearson Education Ltd.
2. Atkins, P. and De Paula, J. (2009) *Atkins' Physical Chemistry*. Oxford University Press.
3. Silbey, R. J. Alberty, R. A. and Bawendi, M. G. (2004)*Physical Chemistry*. Wiley-Interscience Publication.
4. Engel, T. and Reid, P. (2012). *Thermodynamics, Statistical Thermodynamics, and Kinetics*. Pearson Education.
5. Lakowicz, J. R. (2006). *Principles of Fluorescence Spectroscopy*. Springer.
6. Barrow, G. M. (2007) *Physical Chemistry*. Tata McGraw-Hill Publishers.
7. Kapoor, K. L. (2011) *Text Book of Physical Chemistry*.3/5, Macmillan Publishers.
8. McQuarrie, D. A. and Simon, J. D. (1998) *Physical Chemistry: A Molecular Approach*. Viva Books.
9. Moore, J. W., and Pearson, R. G. (1981). *Kinetics and Mechanism*. John Wiley and Sons.
10. Raj, G. (2002). *Surface Chemistry (Adsorption)*. Goel Publishing House.
11. Moore, J. W. and Pearson, R. G. (1981) *Kinetics and Mechanism*. John Wiley and Sons.
12. Puri, B.R., Sharma L.R. and Pathania, M.S. (2013) *Principles of Physical Chemistry*. Vishal Publishing Company.

**Course Title: Spectroscopic Analysis**

**Course Code: CHM.524**

**Total Contact Hours: 45**

L	T	P	Cr
4	0	0	4

**Learning Outcome:** At the end of this course student will be able to

- Identify various spectroscopic techniques (UV, IR, NMR and MS) used in organic synthesis for structure elucidation.
- Predict NMR spectra and various fragment-ions/peaks in MS of a given molecular structure.
- Analyse and interpret the combined spectroscopic data (UV-Vis, IR,  $^1\text{H}$  &  $^{13}\text{C}$  NMR) for structural elucidation of unknown organic molecules.

### **Unit I**

**15 Hours**

**UV-Visible spectroscopy:** Introduction, role of solvents, chromophores and their interaction with UV-visible radiation. Woodward-Fieser rule for conjugated dienes and carbonyl compounds

**Infrared Spectroscopy:** Infrared radiation and its interaction with organic molecules, vibrational mode of bonds, effect of hydrogen bonding and conjugation on absorption bands, interpretation of IR spectra. FTIR.

### **Unit II**

**14 Hours**

**Nuclear magnetic resonance spectroscopy:** Introduction, chemical shift and factors influencing chemical shift, reference standards and solvents. spin-spin coupling, coupling constants, long range coupling, effect of deuteration, integration of signals, interpretation of spectra, spin decoupling, double resonance and shift reagent methods, resonance of other nuclei e.g.  $^{19}\text{F}$ ,  $^{15}\text{N}$ ,  $^{31}\text{P}$ .

### **Unit III**

**15 Hours**

**$^{13}\text{C}$  NMR:** Introduction, Proton coupled and proton decoupled  $^{13}\text{C}$  NMR, nuclear overhauser enhancement (NOE), DEPT techniques, 2D NMR Correlation spectroscopy (COSY), Homo COSY ( $^1\text{H}$ - $^1\text{H}$  COSY), Hetro COSY ( $^1\text{H}$ - $^{13}\text{C}$  COSY, HMQC), long range  $^1\text{H}$ - $^{13}\text{C}$  COSY (HMBC), NOESY.

### **Unit IV**

**16 Hours**

**Mass spectrometry:** Basic principles and brief outline of instrumentation. Ion formation: EI, CI, FAB, MALDI, ESI, metastable ion,  $\alpha$ -cleavage, McLafferty rearrangement, Retro-Diels-Alder cleavage, nitrogen rule, fragmentation process of organic molecules in relation to molecular structure determination. Relative abundance of isotopes, High resolution mass spectrometry (HRMS) and recent advances in mass spectrometry.

Problems for structure elucidation using the above spectroscopic techniques.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

### Suggested Readings

1. Pavia, D. L., Lampman, G. M., Kriz, G. S., and Vyvyan, J. A. (2008). *Introduction to Spectroscopy*. Cengage Learning.
2. Gross, J. H. (2006). *Mass Spectrometry: A Textbook*. Springer Science and Business Media.
3. Banwell, C. N., and McCash, E. M. (1994). *Fundamentals of Molecular Spectroscopy*(Vol. 851). New York: McGraw-Hill.
4. Dyer, J. R. (1965). *Applications of Absorption Spectroscopy of Organic Compounds*. Phi Learning.
5. Kalsi, P. S. (2007). *Spectroscopy of Organic Compounds*. New Age International.
6. Kemp, W. (1998). *Organic Spectroscopy*, ELBS.
7. Khopkar, S. M. (1998). *Basic Concepts of Analytical Chemistry*. New Age International.
8. Melinda, J.D. (2010). *Introduction to Solid NMR Spectroscopy*. Wiley India Pvt Ltd.
9. Mendham, J., Denney, R. C., Barnes, J. D., and Thomas, M. J. K. (2008). *Vogel's Textbook of Quantitative Chemical Analysis*, Dorling Kindersley.
10. Silverstein, R. M., Webster, F. X., Kiemle, D. J., and Bryce, D. L. (2014). *Spectrometric Identification of Organic Compounds*. John wileyand sons.

**Course Title: Molecular Spectroscopy**

**Course Code: CHM.525**

**Total Contact Hours: 45**

L	T	P	Cr
4	0	0	4

**Learning Outcome::**The students will be able to

- Apply microwave, infrared-vibration-rotation Raman and infra-red Spectroscopy for chemical analysis and prediction of molecular structure
- Demonstrate and apply electronic spectroscopy of different elements and simple molecules.
- Explore application of laser spectroscopy and photoelectron spectroscopy in materials and biomaterials.
- Demonstrate and elucidate the physical principles of nuclear magnetic and electron spin resonance spectroscopy.

### Unit I

**14 Hrs**

**Electronic Spectroscopy:** Electronic transition, energy of electronic transition, selection rules, the Franck-Condon principle.

**Microwave Spectroscopy:** Basic principle and instrumentation, classification of molecules, selection rule in microwave spectroscopy, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities of spectral lines, non-rigid rotor, Stark effect, and applications of microwave spectroscopy.

**Unit II****15 Hrs**

**Vibrational Spectroscopy:** Basic principle and instrumentation, Review of harmonic oscillator, Selection rules, vibrational energies of diatomic molecules, zero point energy, force constant and bond strength, anharmonicity, vibration-rotation spectroscopy, Morse potential energy diagram, P, Q, R branches, vibrations of polyatomic molecules, overtones, hot bands and applications.

**Raman Spectroscopy** - Basic principle and instrumentation, Classical and quantum theories of Raman Effect, vibrational-rotational Raman spectra, selection rules, mutual exclusion principle, resonance Raman Spectroscopy, surface enhanced Raman spectroscopy, coherent anti stokes Raman spectroscopy.

**Unit III****15 Hrs**

**Magnetic Resonance Spectroscopy:** Basic principles of NMR and ESR, instrumentation of NMR and ESR, magnetization vector and relaxation, NMR transitions, Bloch equation, relaxation effects and mechanism, effect of quadrupole nuclei, nuclear overhauser effect (NOE), multiple pulse methods, Hyperfine splitting in ESR.

**Unit IV****16 Hrs**

**Lasers and Laser Spectroscopy:** Principles of laser action, pulsed lasers, examples of lasers: He-Ne, Nd-YAG, dye lasers.

**Photoelectron spectroscopy:** Basic principle and instrumentation, The photoelectric effect, UV photoelectron spectroscopy UPES, X-ray photoelectron spectroscopy XPES.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

**Suggested Readings**

1. Hollas, J. M. (2004). *Modern Spectroscopy*. John Wiley and Sons.
2. Lakowicz, J. R. (2006). *Principles of Fluorescence Spectroscopy*. Springer.
3. Barrow, G. M. (2007) *Physical Chemistry*. Tata McGraw-Hill Publishers.
4. Banwell, C. N., and McCash, E. M. (1994). *Fundamentals of Molecular Spectroscopy* (Vol. 851). New York: McGraw-Hill.
5. Carrington, A., and McLachlan, A. D. (1967). *Introduction to Magnetic Resonance: With Applications to Chemistry and Chemical Physics*. Chapman and Hall, London.
6. Lynden-Bell, R. M., and Harris, R. K. (1969). *Nuclear Magnetic Resonance Spectroscopy*. Appleton-Century-Crofts.
7. Reilley, C. N., Everhart, D. S., and Ho, F. F. L. (1982). *Applied Electron Spectroscopy for Chemical Analysis. Chemical Analysis, 63, 105*. John Wiley.
8. Chang, R. (1971). *Basic Principles of Spectroscopy*. McGraw-Hill.
9. Ghosh, P. K. (1983). *Introduction to Photoelectron Spectroscopy*. John Wiley and Sons, New York.

10. Günther, H. (2013). *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*. John Wiley and Sons.

**Course Title: Practical Inorganic Chemistry –II**

**Course Code: CHM.526**

**Total Contact Hours: 60**

L	T	P	Cr
0	0	4	2

**Learning Outcome:** The students will be able to

- Prepare and purify of different inorganic complexes.
  - Explore various application of UV-Vis, FT-IR, Magnetic moment measurement, Conductivity measurements, NMR and Thermogravimetric analysis for characterization of coordination complexes.
1. Preparation of Chloropentaammine cobalt (III) chloride and its IR measurements.
  2. Preparation of  $[\text{Co}(\text{en})_2\text{Cl}_2] \text{Cl}$ ,  $\text{Na}_2 [\text{Fe}(\text{CN})_5 \text{NH}_3] \cdot \text{H}_2\text{O}$ ,  $\text{Cu}_2(\text{CH}_3\text{COO})_4 (\text{H}_2\text{O})_2$ .
  3. Preparation of  $\text{Hg}[\text{Co}(\text{CNS})_4]$  and used as standard for the magnetic moment measurement
  4. Preparation of cis-and trans- $\text{K} [\text{Cr} (\text{C}_2\text{O}_4)_2 (\text{H}_2\text{O})_2]$  and its IR study.
  5. Preparation of bis(2,4-pentanedione)vanadium(IV) acetate and its piperidine or pyridine complex. Study of both the complexes with the help of infrared, UV-vis spectroscopy and magnetic susceptibility.
  6. Preparation of lead tetraacetate.
  7. Preparation of noble metals(Cu, Ag, Au etc) nanoparticles
  8. Preparation and separation of isomers of  $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]$ , Cu(II) and Ni(II) complexes of Schiff base.
  9. Determination of Chlorophyll content
  10. Determination of gross calorific value (GCV) for fuels.
  11. Determination of pour point, flash point and cloud point of liquid fuel.

**Mode of Transactions:** Demonstration, Experimentation, handling instruments, Explanation of data

**Suggested Readings**

1. Pass, G. and Sutcliffe H. (1979). *Practical Inorganic Chemistry*. Chapman and Hall Ltd.
2. Nakamoto, K. (1997). *Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A and B*. John Wiley and Sons,.
3. Mendham, J., Denney, R.C., Barnes, J.D. and Thomas, M. J. K. (2000). *Vogel's Textbook of Quantitative Chemical Analysis*, Pearson Education Ltd.
4. Kolthoff, I. M., and Sandell, E. B. (1944). *Text Book of Quantitative Inorganic Analysis*. The Macmillan; New york.

5. Marr, G., and Rockett, B. W. (1960). *Practical Inorganic Chemistry*. John Wiley and Sons.
6. Jolly, W.L. (1961). *Synthetic Inorganic Chemistry*. Prentice Hall, Inc.

**Course Title: Practical Physical Chemistry-II**

**Course Code: CHM.527**

**Total Contact Hours: 60**

L	T	P	Cr
0	0	4	2

**Learning Outcome:**

The students will be able to

- Develop and gain various experimental skills on conductivity meter, potentiometer, pH meter, viscometer, refractometer, spectrophotometer, CD, DSC, DLS and FTIR for different applications.
1. Determination of behavior and strength of a given acid/base by titrating with an base/acid conductometrically.
  2. Determination of solubility and solubility product of sparingly soluble salts (e.g.,  $\text{PbSO}_4$ ,  $\text{BaSO}_4$ ) conductometrically.
  3. Determination of Critical Micellar Concentration (CMC) of CTAB and SDS using conductometric method.
  4. Determination standard electrode potential of  $\text{Fe}^{2+}/\text{Fe}^{3+}$  system by potentiometer using potassium permanganate solution.
  5. Determination standard electrode potential of  $\text{Fe}^{2+}/\text{Fe}^{3+}$  system by potentiometer using ceric ammonium nitrate solution.
  6. Determination of  $\text{pK}_a$  of acetic acid and  $\text{H}_3\text{PO}_4$  by potentiometric titration using NaOH.
  7. Determination of stability constant for Cu(II)-glycinate complex using potentiometry.
  8. Determination of relative and absolute viscosity of a given liquid.
  9. Determination of surface tension of alcohols.
  10. Determination of refractive indices (RI) of given liquids and determination of the concentration from RI.
  11. Verification of the Lambert Beer's law.
  12. Determination of concentrations of proteins and DNA using spectrophotometer
  13. Preparation of buffers and measurement of their pH.
  14. Structural analysis of amino acids and proteins using CD and Fluorescence spectrometer.
  15. Study of thermal denaturation ( $T_m$  and  $\Delta H_m$ ) of proteins and DNA using UV-Visible spectrophotometer, CD spectrometer and DSC.
  16. Study of chemical of proteins and DNA using UV-Visible and CD spectrometer.
  17. Molecular weight of a non-electrolyte by cryoscopy method.



18. Determination of mean, median, standard errors, standard deviation, coefficient of variance using software.
19. Measurement of zeta potential and sizes of nanoparticles by DLS

**Mode of Transactions:** Demonstration, Experimentation, handling instruments, Explanation of data

### Suggested Readings

1. Nad, A. K., Mahapatra, B. and Ghoshal, A. (2014). *An Advanced Course in Practical Chemistry*. New Central Book Agency (P) Ltd.
2. Maity S., and Ghosh, N. (2012). *Physical Chemistry Practical*. New Central Book Agency (P) Ltd.
3. Elias, A. J. (2002). *A Collection of Interesting General Chemistry Experiments*. Universities Press.
4. Khosla, B.D., Garg, V.C., and Gulati A.R. (2007). *Senior Practical Physical Chemistry*. S. Chand and Sons.
5. Yadav, J. B. (2006). *Advanced Practical Physical Chemistry*. Krishna Prakashan Media.
6. Das, R. C., and Behera, B. (1983). *Experimental Physical Chemistry*. Tata McGraw-Hill.
7. Das, R.C., and Behra, B. (1983). *Experimental Physical Chemistry*. 1983, Tata McGraw-Hill.
8. James, A. M., and Prichard, F. E. (1974). *Practical Physical Chemistry*. New York: Longman.
9. Ghosh, J.C. (1990). *Experiments in Physical Chemistry*, Bharati Bhavan.

**Course Title: Seminar**

**Course Code: CHM.542**

**Total Contact Hours: 15**

L	T	P	Cr
0	0	0	1

**Learning Outcome:** The student would be able to

- Investigate various aspects related to the chemistry problem.
- Appreciate the literature and its relevance to his/her topic of interest
- Technical write and presentation the chemical problem in hand.
- Should generate interest in current topics of research and commercial worth of chemistry.

Seminar would emphasize on problem solving approach and use of various techniques to prove a chemical process /techniques. The seminar would emphasize upon the writeup of introduction, review of literature and cited references. The presentation would promote the use of graphical features of MS-Office and Chemdraw,® apart from spreadsheets and imaging software

**Course Title: Protein Chemistry**

**Course Code: CHM.558**

**Total Contact Hours: 15**

L	T	P	Cr
1	0	0	1

**Learning Outcome:** The students will acquire knowledge of

- Structure and biological functions of proteins.
- The role of metals in biology
- Mechanism of protein folding
- Understanding of causes and treatment of neurodegenerative, iron metabolic disorder and diabetes.

**Unit: I**

Buffers; Amino Acids; Proteins: Function and Structure, Protein synthesis; Protein engineering and protein/protein interactions.

**Unit: II**

Structure and function of hemoglobin, myoglobin and transferrin; Iron metabolic disorders (anemia, Sickle cell anemia, thalassemia, hemochromatosis), Diabetes; Types of diabetes and its causes/prevention/treatment, Interlink between iron metabolic disorder and diabetes; Cancer and its causes/treatments.

**Unit III.** Protein folding and misfolding, Determination of protein structures and folding intermediates; In vitro analyses of off-pathway aggregation and amyloid formation; Key chaperones and chaperonins;

**Unit IV.** Practical implications in biotechnology; Special emphasis on human protein deposition diseases including Alzheimer's, Parkinson's and Huntington's disease.

**Mode of Transactions:** Demonstration, Experimentation, handling instruments, Explanation of data

**Suggested Readings**

1. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic chemistry: principles of structure and reactivity*. Pearson Education India.
2. Douglas, B. E., and McDaniel, D. H. (1965). *Concepts and models of inorganic chemistry*. John Wiley and Sons.
3. Cotton, F. A., and Wilkinson, G. (1988). *Advanced inorganic chemistry* (Vol. 545). New York: Wiley.
4. Elschenbroich, C. (2016). *Organometallics*. John Wiley and Sons.
5. Atkins, P., Overton, T., Rourke, J., Weller, J., and Armstrong, F., (2010). *Shriver and Atkins' inorganic chemistry*. Oxford University Press.

## SEMESTER III

**Course Title: Inorganic Chemistry-III**

**Course Code: CHM.551**

**Total Contact Hours: 60**

L	T	P	Cr
4	0	0	4

**Learning Outcome:** The students will be able to

- Details on f-block elements properties
- Structural support to inorganic compounds through spectroscopic techniques
- Understanding the nuclear behaviour of various nucleoids.

### Unit I

**15 Hours**

**Lanthanides, actinides and super-heavy elements:** Coordination chemistry, magnetic and spectral properties, comparison of general properties of lanthanides and actinides, comparison with d-block elements, organolanthanides and actinides, analytical application of lanthanides and actinides-lanthanides as shift reagents and high temperature super conductors.

### Unit II

**15 Hours**

**Nuclear Magnetic Resonance (NMR) and Electron Spin Resonance (ESR) Spectroscopy:**

**NMR:** Basic concepts of NMR with emphasis on  $^{31}\text{P}$ ,  $^{19}\text{F}$ ,  $^{29}\text{Si}$ ,  $^{11}\text{B}$ ,  $^{10}\text{B}$ ,  $^{57}\text{Se}$ ,  $^{125}\text{Te}$ ,  $^{95}\text{Mo}$ ,  $^{109}\text{Ag}$ ,  $^{195}\text{Pt}$ ,  $^{119}\text{Sn}$  and an explanations with appropriate examples. NMR study in Fluxional organometallic compounds.

**ESR:** Basic elements of ESR, Fine structure of ESR Signal transition metal ions, Zero-field Splitting, Kramer's Degeneracy, Hyperfine Splitting of various free radical spin polarization for atoms and transition metal ions, spin orbit coupling and significance of  $g$ -tensors, application of transition metal complexes (having one unpaired electron) including biological systems.

### Unit III

**15 Hours**

**Mossbauer Spectroscopy:** Basic principles, spectral parameters and spectrum display, application of the technique to the studies of (1) bonding and structures of  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  compounds including those of intermediate spin, (2)  $\text{Sn}^{2+}$  and  $\text{Sn}^{4+}$  compounds- nature of M-L bond, coordination number, structure and (3) detection of oxidation state and non-equivalent MB atoms.

### Unit IV

**15 Hours**

**Nuclear Chemistry:** Classification of nuclides, nuclear stability, atomic energy, types of nuclear reactions-fission and fusion, nuclear decay laws, radioanalytical techniques.

**Mode of Transactions:** Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brain storming, Tutorial

### Suggested Readings

1. Cotton, F.A. and Lippard, S.J., (1998). *Progress in Inorganic Chemistry*. Vol. 8, Wiley Internationals.
2. Lever, A.B.P.,(1984). *Inorganic Electronic Spectroscopy*. Elsevier Science Publishers B.V.
3. Parish, R.V.,(1990). *NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry*. Ellis Harwood.
4. Silverstein, R.M., Bassler, G.C.,andMorrill, T.C. (2002). *Spectrometric Identification of Organic Compounds*. John Wileyand Sons.
5. Abraham, R. J., Fisher, J., and Loftus, P. (1988). *Introductionto NMR spectroscopy*. Wiley.
6. Martin, M. L., Delpuech, J. J., and Martin, G. J. J. (1980). *Practical NMR spectroscopy*. Heyden.
7. Williams, D. H., and Fleming, I. (1980). *Spectroscopic Methods in Organic Chemistry*. McGraw-Hill.
8. Greenwood, N. N., and Earnshaw, A. (2012). *Chemistry of the Elements*. Elsevier.

**Course Title: Organic Chemistry-III**

**Course Code: CHM.552**

**Total Contact Hours: 60**

L	T	P	Cr
4	0	0	4

**Learning Outcome:** The students will be able to

- Identify various retrosynthetic strategies and designing the synthesis of target molecules.
- Explore various oxidizing and reducing reagents in a logical manner for their application in functional group conversion in organic synthesis.
- Compare the reactivity of smaller, five and six membered heterocyclic compounds.

#### Unit I

**14 Hours**

**Retrosynthesis:** Synthons, synthetic equivalent, functional group interconversion (FGI), functional group addition, functional group elimination, criteria for selection of target, linear and convergent synthesis, retrosynthetic analysis involving chemoselectivity, reversal of polarity (umpolung), importance of the order of events in organic synthesis. One group and two group C-X disconnections, two group C-C disconnections; Diels-Alder reaction, control in carbonyl condensation.

#### Unit II

**15 Hours**

**Metal and non-metal mediated oxidation:** Mechanism, selectivity, stereochemistry and applications of oxidation reactions, Baeyer-Villiger, Oppenauer oxidation, oxidation reactions using DDQ, NBS, Pb(OAc)<sub>4</sub>, Selenium dioxide, PCC, PDC, Cr and Mn based reagents, phase transfer catalysis, Periodic

acid, Ceric ammonium nitrate, OsO<sub>4</sub>, Swern oxidation, hydroboration, Sharpless asymmetric epoxidation, epoxidations using peracids. Recent approaches for oxidation using green oxidants.

### Unit III

15 Hours

**Metal and non-metal mediated reduction:** Mechanism, selectivity, stereochemistry and applications of catalytic hydrogenations using Pd, Pt and Ni catalysts (Lindlar, Rosenmund, Adam's catalysts), Wilkinson's catalysis, Clemmensen reduction, Wolff-Kishner reduction, Meerwein-Ponndorf-Verley reduction, dissolving metal reductions, Birch reduction, Reductions using metal hydride NaBH<sub>4</sub>, Luche reduction NaBH<sub>3</sub>CN, L-selectride, K-selectride, NaBH(OAc)<sub>3</sub>, LiAlH<sub>4</sub>, DIBAL.

### Unit IV

16 Hours

**Heterocyclic Chemistry:** Systematic (Hantzsch-Widman system) and replacement nomenclature for monocyclic, fused and bridged heterocycles, aromatic heterocycle, non-aromatic heterocycle: bond angle and torsional strains and their consequences in small ring heterocycles, conformation of six-membered heterocycles.

**Three-membered and four-membered heterocycles:** aziridines, oxiranes, thiranes, azetidines, oxetanes.

**Five membered heterocycles containing two heteroatoms (S,N,O):** Diazoles (imidazole, pyrazole), triazoles, oxazoles and thiazoles.

**Benzo-fused five-membered heterocycles:** Indoles, benzofurans and benzimidazoles.

**Six-membered heterocycles:** Synthesis and reactions of coumarins, chromones.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

### Suggested Readings

1. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*. Narosa Publishing House (P) Ltd., New Delhi.
2. Bansal, R. K. (2012). *A Textbook of Organic Chemistry*. New Age International.
3. Bansal, R.K. *Heterocyclic Chemistry*, 5<sup>th</sup> Edition, 2010, New Age International (P) Ltd., New Delhi.
4. Carey, F. A., and Sundberg, R. J. (2007). *Advanced organic chemistry: part B*. Springer Science and Business Media.
5. Finar, I. L. (1996). *Textbook of Organic Chemistry*. ELBS, Pearson Education UK.
6. Gilchrist, T.L., (1997). *Heterocyclic Chemistry*. Addison Wesley Longman Publishers, US.
7. Gupta R.R., Kumar M., and Gupta V., (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles*. Vol. 1-3, Springer Verlag, India.

8. Joule, J.A.,and Mills, K.,(2010). *Heterocyclic Chemistry*.Blackwell Publishers, New York.
9. Smith, M. B.,(2013). *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*.John Wiley and Sons.
10. Warren, S., (2010). *Organic synthesis: The Synthon Approach*. John Wileyand Sons.
11. Warren, S.,andWyatt, P., (2010).*Designing Organic synthesis: A Disconnection Approach*. John Wiley and Sons.
12. Corey, E.J.,and Cheng X.-M., (1989).*The Logic of Chemical Synthesis*. John Wiley and Sons.

**Course Title: Bio-inorganic and Biophysical Chemistry**

**Course Code: CHM.553**

**Total Contact Hours: 45**

L	T	P	Cr
3	0	0	3

**Learning Outcome:** At the end of this course student will be able to

- Determined structure and biological functions of metalloproteins and enzymes.
- Classify of metallobiomolecules on the basis of their functional properties.
- Know the role of metals in biology
- Determined the factors that govern the thermodynamic and mechanical stability, folding, and dynamics of proteins.
- Work on the kinetics, thermodynamics, and mechanism of protein folding.

### **Unit I**

**11 Hours**

**Inorganic Chemistry of Enzymes – I:** Metalloporphyrins: Hemoglobin and myoglobin, nature of heme-dioxygen binding, model systems, cooperativity in hemoglobin, structure and function of hemoglobin and myoglobin. Other iron-prophyrin biomolecules, peroxidases and catalases, cytochromes, cytochrome P450 enzymes, other natural oxygen carriers, hemerythrins, electron transfer. Biochemistry of iron, iron storage and transport, ferritin, transferrin.

### **Unit II**

**12 Hours**

**Inorganic Chemistry of Enzymes – II:** Metallothioneins: Ferridoxins, carboxypeptidase, carbonicanhydrase, blue copper proteins, superoxide dismutase, hemocyanines.

**Enzymes:** Structure and function, inhibition and poisoning vitamin B<sub>12</sub> and B<sub>12</sub> coenzymes metallothioneins, bio-inorganic chemistry of Mo and W.

### **Unit III**

**11 Hours**

**Metal Ions in Biological Systems:** Role of metal ions in replication and transcription process of nucleic acids. Biochemistry of calcium as hormonal messenger, muscle contraction blood clotting, neurotransmitter, metals in the regulation of biochemical events.

## Unit IV

11 Hours

**Biophysical Chemistry:** Principles of biophysical chemistry (pH, buffer, reaction kinetics, thermodynamics), physical principle of structure, function, and folding of proteins, conformations of proteins (Ramachandran plot, secondary, tertiary and quaternary structure; domains; motif and folds), determination of protein structures by spectroscopic methods (CD, FTIR, NMR), thermodynamics of protein folding by spectroscopic and calorimetric methods, protein conformational study by NMR and fluorescence spectroscopy.

**Mode of Transactions:** Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brain storming, Tutorial

### Suggested Readings

1. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic chemistry: principles of structure and reactivity*. Pearson Education India.
2. Douglas, B. E., and McDaniel, D. H. (1965). *Concepts and models of inorganic chemistry*. John Wiley and Sons.
3. Cotton, F. A., and Wilkinson, G. (1988). *Advanced inorganic chemistry* (Vol. 545). New York: Wiley.
4. Elschenbroich, C. (2016). *Organometallics*. John Wiley and Sons.
5. Atkins, P., Overton, T., Rourke, J., Weller, J., and Armstrong, F., (2010). *Shriver and Atkins' inorganic chemistry*. Oxford University Press.
6. Cowan, J.A. (1997). *Inorganic Biochemistry: An Introduction*. Wiley – VCH.
7. Lippard, S. J. (1991). *Progress in Inorganic Chemistry*. Vol. 18, Wiley-Interscience.
8. Lippard, S. J. (1991). *Progress in Inorganic Chemistry*. Vols. 38, Wiley-Interscience.
9. Lesk, A.M., (2010). *Introduction to Protein Science: Architecture, Function, and Genomics*. Oxford University Press.
10. Cantor, C.R. and Schimmel, P.R., (1980). *Biophysical Chemistry*. Freeman.
11. Van Holde, K.E., Johnson, W.C., and Ho, P.S., (2006). *Principles of Physical Biochemistry*. Pearson Education.
12. Harding, S.E. and Chowdhry, B. Z. (2001). *Protein-Ligand Interactions*. Oxford University Press.

**Course Title: Practical Organic Chemistry-III****Course Code: CHM.554****Total Contact Hours: 60**

L	T	P	Cr
0	0	4	2

**Learning Outcome:** At the end of this course students will be able to

- Identify various agents used for drying of solvents and their disposal.
- Separate and purify the desired product from an organic reaction.
- Characterize organic compounds using various spectroscopic techniques.
- Realise the impact of various coupling and click chemistry strategies for construction of value added chemicals.

**Experiments:****Solvent Drying:** Use of sodium metal for drying of toluene and precautions while quenching the residual sodium. Drying of DCM using  $P_2O_5$  and safe disposal of residual  $P_2O_5$ .

1. **Synthesis:** Separation and purification of organic compounds by column chromatography, percentage yield calculation (any seven)
  1. Preparation of allylic alcohols *via* Baylis-Hillman reaction using DABCO as a catalyst and their characterization through various spectroscopic techniques.
  2. To study the reaction of vanillin with malonic acid for the synthesis of 4- Vinylguaiaicol.
  3. To synthesise *p*-iodonitrobenzene from *p*-nitroaniline.
  4. To study Buchwald-Hartwig reaction of aryl halide with an amine using Cu-based catalyst.
  5. Synthesis of triazole *via* reaction of phenylacetylene with azide (Huisgen cycloaddition).
  6. Synthesis of stilbenes *via* Heck coupling Strategy.
  7. To study decarboxylation of Ferulic acid under microwave irradiation.
  8. Synthesis of imidazolium and pyridinium based ionic liquids.
  9. To study dehydration of benzylic alcohols using imidazolium based ionic liquid.
  10. To synthesize benzofused heterocyclic compounds (any one)
    - (i) Coumarin (ii) benzothiazole
  11. To synthesize 2-phenyl-1,3,4-oxadiazole from benzhydrazide.
  12. To synthesize substituted benzodiazepine from chalcone *via* reflux conditions.
  13. Synthesis of benzothiazole starting from 2-aminothiophenol.
  14. To study amination of benzothiazole with amines.
  15. Synthesis of bromohydrin using NBS from phenylpropene
  16. To study synthesis of Dilantin *via* benzylic-acid rearrangement
  17. To study the rearrangement of benzopinacol into benzopinacolone
  18. To study the three component coupling for the synthesis of (any one)
    - (i) dihydropyrimidinone (*via* Bignelli reaction)
    - (ii) propargylamine (*via*  $A^3$ -coupling)



**Mode of Transactions:** Demonstration, PPT, videos, Lecture cum demonstration

**Suggested Readings**

1. Harwood, L.M. and Moody, C.J. (1989) *Experimental Organic Chemistry*. Blackwell Scientific Publishers.
2. Vogel, A.I. (1978) *Textbook of Practical Organic Chemistry*. ELBS, Longman Group Ltd.
3. Mann, F.G. and Saunders, B.C. (1975) *Practical Organic Chemistry*. Orient Longman Pvt. Ltd.
4. Leonard, J. and Lygo, B. (1995) *Advanced Practical Organic Chemistry*. Chapman and Hall,.
5. Armarego, W.L. and Chai, C. (2012) *Purification of Laboratory Chemicals*. Butterworth-Heinemann.
6. Young, J.A. (1991) *Improving Safety in the Chemical Laboratory: A Practical Guide*. Wiley Publishing.

**Course Title: Practical Physical Chemistry-III**

**Course Code: CHM.555**

**Total Contact Hours: 60**

L	T	P	Cr
0	0	4	2

**Learning Outcome:** The students will be able to

- Become expert in various experimental techniques for controlling the chemical reactions.
- Measure of various physical and chemical properties.
- Apply related experiments for their research work.

**Experiments:**

1. To verify Freundlich and Langmuir adsorption isotherms for adsorption of acetic acid on activated charcoal.
2. Determination of partition coefficient of benzoic acid between organic solvent and water.
3. Determination of partition coefficient of iodine between water and octanol and determination of equilibrium constant of tri-iodide.
4. Determination of rate constant of hydrolysis of an ester and to study the effect of ionic strength on reaction rate.
5. To study kinetics of inversion of cane sugar by optical rotation measurement.
6. Determination of activation energy of a reaction by spectrophotometer.
7. Energy of activation of acid catalyzed hydrolysis of methyl acetate.
8. Kinetics of acid-catalysed reaction between acetone-iodine
9. Determination of order of  $S_2O_8^{2-} + I^- \rightarrow SO_4^{2-} + I_2$  reaction
10. Determination of energy of activation of  $S_2O_8^{2-} + I^- \rightarrow SO_4^{2-} + I_2$  reaction

11. Studies on the effect of variation of ionic strength on the rate of  $S_2O_8^{2-} + I^- \rightarrow SO_4^{2-} + I_2$  reaction
12. Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine clock reaction.
13. Curve fitting using linear and non-linear (Activation thermodynamic parameter, equilibrium thermodynamic parameter) regression analysis using software.
14. Determination of stability constant of Fe(III)-salicylic acid complex by spectrophotometer.
15. Determination of Michaelis-Menten ( $K_m$ ) constant in enzyme kinetics.
16. Particle size and hydrodynamic radii analysis for adsorbents, protein or nanoparticles
17. Measurement of affinity constant of metal complex or metal binding to protein by ITC

### Suggested Readings

1. Nad, A. K., Mahapatra, B. and Ghoshal, A. (2014). *An Advanced Course in Practical Chemistry*. New Central Book Agency (P) Ltd.
2. Maity S., and Ghosh, N. (2012). *Physical Chemistry Practical*. New Central Book Agency (P) Ltd.
3. Elias, A. J. (2002). *A Collection of Interesting General Chemistry Experiments*. Universities Press.
4. Khosla, B.D., Garg, V.C., and Gulati A.R. (2007). *Senior Practical Physical Chemistry*. S. Chand and Sons.
5. Yadav, J. B. (2006). *Advanced Practical Physical Chemistry*. Krishna Prakashan Media.
6. Das, R. C., and Behera, B. (1983). *Experimental Physical Chemistry*. Tata McGraw-Hill.
7. Das, R.C., and Behra, B. (1983). *Experimental Physical Chemistry*. 1983, Tata McGraw-Hill.
8. James, A. M., and Prichard, F. E. (1974). *Practical Physical Chemistry*. New York: Longman.
9. Ghosh, J.C. (1990). *Experiments in Physical Chemistry*, Bharati Bhavan.

**Mode of Transactions:** Demonstration, PPT, videos, Lecture cum demonstration

**Course Title: Research Methodology**

**Course Code: CHM.556**

**Total Lecture: 30**

L	T	P	Cr
2	0	0	2

**Learning Outcome:** At the end of this course student will be able to

- Design research problem.
- Know why educational research is undertaken, and the audiences that profit from research studies.

- Identify the overall process of designing a research study
- Familiar with ethical issues in educational research, including those issues that arise in using quantitative and qualitative research.

### **Unit I**

**8 Hours**

**General principles of research:** Meaning and importance of research, Critical thinking, Formulating hypothesis and development of research plan, Review of literature, Interpretation of results and discussion.

**Bibliographic index and research quality parameters:** citation index, impact factor, *h* index, i10 index, etc. Research engines such as google scholar, Scopus, web of science, etc

### **Unit II**

**8 Hours**

**Technical and scientific writing:** Technical and Scientific writing - theses, technical papers, reviews, electronic communication, research papers, etc., Poster preparation and Presentation and Dissertation. Reference Management using various softwares such as Endnote, reference manager, Refworks, etc. Communication skills—defining communication; type of communication; techniques of communication, etc.

### **Unit III**

**7 Hours**

**Library:** Classification systems, e-Library, Reference management, Web-based literature search engines.

### **Unit IV**

**7 Hours**

**Plagiarism:** Plagiarism, definition, Search engines, regulations, policies and documents/thesis/manuscripts checking through softwares, Knowing and Avoiding Plagiarism during documents/thesis/manuscripts/ scientific writing.

**Mode of Transactions:** Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brain storming, Tutorial

### **Suggested Readings:**

1. Gupta, S. (2005). *Research Methodology and Statistical Techniques*. Deepand Deep Publications (p) Ltd.
2. Kothari, C. R. (2008.) *Research Methodology(s)*. New Age International (p) Limited.
3. Web resources: [www.sciencedirect.com](http://www.sciencedirect.com) for journal references, [www.aip.org](http://www.aip.org) and [www.aps.org](http://www.aps.org) for reference styles.
4. Web resources: [www.nature.com](http://www.nature.com), [www.sciencemag.org](http://www.sciencemag.org),  
[www.springer.com](http://www.springer.com), [www.pnas.org](http://www.pnas.org), [www.tandf.co.uk](http://www.tandf.co.uk),  
[www.opticsinfobase.org](http://www.opticsinfobase.org) for research updates.

**Course Title: Current Trends in Organic Synthesis**

**Course Code: CHM.579**

**Total Contact Hours: 45**

L	T	P	Cr
3	0	0	3

**Learning Outcome:** At the end of this course student will be able to

- Know the potential of free radical chemistry for various coupling reactions including metal free C-H bond activation/functionalization
- Apply the concept of enolate chemistry for controlling the selectivity of various organic transformations.
- Design various processes for the synthesis commercially important molecules taking into consideration the protection and deprotection strategies.

### **Unit I**

**11 Hours**

**Free radical reactions:** Types of free radical reactions, free radical substitution mechanism at an aromatic substrate, free radical rearrangement, neighbouring group assistance, reactivity for aliphatic and aromatic substrates at a bridgehead, Reactivity in the attacking radicals, the effect of solvents on reactivity, auto-oxidation. Coupling of alkynes and arylation of aromatic compounds by diazonium salts. Recent trends in oxidative functionalization of C-H bond *via* free radical chemistry.

### **Unit II**

**11 Hours**

**Enolate Chemistry:** Regio- and stereo-selectivity in enolate generation. "O" versus "C" alkylation, effect of solvent, counter-cation and electrophiles; symbiotic effect; thermodynamically and kinetically controlled enolate formations; various transition state models to explain stereoselective enolate formation; enamines and metallo-enamines; regioselectivity in generation, application in controlling the selectivity of alkylation.

### **Unit III**

**11 Hours**

**Protection and deprotection of various functional groups:** Protection of alcohols by ether, silyl ethers and ester formations and their deprotection, protection of carbonyls by acetal and ketal formation and their deprotection, protection of 1, 2 diols- by acetal, ketal and carbonate formation and their deprotection, protection of amines by acetylation, benzylation, benzyloxy carbonyl, *t*-butoxycarbonyl (Boc), fmoc, triphenyl methyl groups and their deprotection, protection of carboxylic acids by ester formation and their deprotection: Recent advances in protection-deprotection free organic synthesis.

### **Unit IV**

**12 Hours**

**New synthetic reactions:** Baylis-Hillman reaction, Biginelli reaction, Mukaiyama aldol reaction, Mitsunobu reaction, McMurrey reaction, Julia-Lythgoe olefination, and Peterson's stereoselective olefination, Buchwald-Hartwig coupling, Eishenmosher-Tanabe fragmentation and Shapiro reaction,

Stork-enamine reaction, Aza-Cope, Aza-Wittig reaction, Ugi reaction, Robinson-Gabriel synthesis, Vilsmeier-Haack reaction.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

### Suggested Readings

1. Finar, I.L., (2012). *Organic Chemistry Vol. 1*. Pearson Education, UK.
2. Finar, I.L., (2012). *Organic Chemistry Vol. 2: Stereochemistry and the Chemistry of Natural Products*. Pearson Education, UK.
3. Fleming I., (2011). *Molecular Orbitals and Organic Chemical Reactions*. John Wiley and Sons.
4. Li, J. J., (2014). *Name Reactions: A Collection of Detailed Reaction Mechanism*. Springer-Verlag.
5. Kalsi, P.S. (2010). *Organic Reactions and Their Mechanisms*. New Age International Pub.
6. McMurry, J. (1996). *Organic Chemistry*, Brooks Cole.
7. Mukherjee, S.M., and Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd.
8. Smith, M. B., (2013). *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*. John Wiley and Sons.
9. Solomon, T.W.G., Fryhle, C.B. and Snyder, S. A., (2013). *Organic Chemistry*. John Wiley and Sons, Inc.
10. Sykes, P. A. (1997). *Guide Book to Mechanism in Organic Chemistry*. Prentice Hall.
11. Carruthers, W. (2004). *Some Modern Methods of Organic Synthesis*. Cambridge Uni. Press, UK.

**Course Title: Basic Instrumentation and Sensors**

**Course Code: CHM.557**

**Total Contact Hours: 15**

L	T	P	Cr
1	0	0	1

**Learning outcome:** The student will be able to

- Apply various instruments for his routine analysis in research undertake in project.
- Know the intricacies and maintenance of the equipments.

### Unit I

**Light as a source of Analysis:** UV-Visible Spectroscopy, FTIR Spectroscopy, Fluorescence spectroscopy, Basic Microscopy, Fluorescence and Confocal Laser Scanning Microscopy and Fluorescence correlation spectroscopy.

## Unit II

**Surface Analysis:** Scanning Electron Microscope, Atomic Force Microscopy, Scanning Tunneling Microscopy, Transmission Electron Microscopy, X-Ray diffraction, Photoelectron Spectroscopy (UPE, XP and Auger Spectroscopy), RHEED, SAED, LEED.

## Unit III

**Alternate Method of Analysis:** Principles and construction of potentiometry and biochemical analyzers, Ion selective electrodes, DO-meter.

**Sensors:** Concept of sensors and actuators, receptors, transducers, optical sensors, SERS and MEMS, applications to biomedical, chemical and industrial processes.

## Unit IV

**Chromatography:** General principle of chromatography, sample preparation in chromatography for volatile and non-volatile components, partition co-efficients, liquid-liquid and solid-liquid partition, Solid phase extractions and materials for SPE, application of derivatizations for pre and post column analysis, rational selection of columns and column chemistry.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

## Suggested Readings

1. Skoog, D. A., Holler, F. J., and Crouch, S. R. (2017). *Principles of Instrumental Analysis*. Cengage learning.
2. Willard, H. H., Merritt Jr, L. L., Dean, J. A., and Settle Jr, F. A. (1988). *Instrumental Methods of Analysis*. CBS Publishers.
3. Christian, G. D. (1994). *Analytical Chemistry*. John Wiley and Sons, USA, 331.
4. Turner, A., Karube, I., and Wilson, G. S. (1987). *Biosensors: Fundamentals and Applications*. Oxford university press.
5. Janata, J. (2010). *Principles of Chemical Sensors*. Springer Science and Business Media.

**Course Title: Project**

**Course Code: CHM.599**

**Total Contact Hours: 180**

L	T	P	Cr
0	0	0	6

**Learning Outcome:** The student would be able to

- Investigate various aspects related to the chemistry problem.
- Appreciate the literature and its relevance to his topic of interest
- Write synopsis independently
- Would generate interest in current topics of research.

Project supervisor would be allocated at the start of the semester and research project would be undertaken in discussion with the project supervisor. At the end of the semester the student has to prepare a project report as per the university guidelines. Upon submission of the project report, the projects would be evaluated based on a project presentation.

## SEMESTER IV

**Course Title: Concepts in Chemistry-I**

**Course Code: CHM.572**

**Total Contact Hours: 30**

L	T	P	Cr
2	0	0	2

**Learning Outcome:** This course is designed to exercise various problems in organic synthesis so that students can compete for national level competitive examinations such as UGC-CSIR-NET, GATE etc. After completion of this course student will be able to

- Interpret spectroscopic data and solve various problems of structure elucidation.
- Identify the product of various pericyclic reactions including stereoselective aspects of various organic transformations.
- Compare the reactivity of various heterocyclic compounds and utility of natural products.

### Unit I

**7 Hours**

**Combined Structure problems:** Exercises of structure elucidation of unknown compounds *via* combined spectral interpretation of IR, UV-vis,  $^1\text{H}$  and  $^{13}\text{C}$  NMR and mass spectra, along with two-dimensional NMR spectroscopy. IUPAC nomenclature of organic molecules including regio- and stereoisomers.

### Unit II

**7 Hours**

**Organic reaction mechanisms:** involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways.

Various strategies for asymmetric synthesis and its applications in natural products and drug molecules.

### Unit III

**8 Hours**

**Organic transformations and reagents:** Functional group interconversion including oxidations and reductions; common catalysts and reagents: organic, inorganic, organometallic and enzymatic. stereoselective transformations. Green catalysts in organic synthesis. Exercises on stereochemical aspects of various pericyclic reactions.

**Unit IV****8 Hours**

Reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S) and their utility in organic synthesis. Chemistry of natural products: Carbohydrates, proteins and peptides, fatty acids, terpenes and alkaloids.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

**Suggested Readings**

1. Pavia, D.L., Lampman, G. M., Kriz, G. S., and Vyavan, J. R., (2010). *Introduction to Spectroscopy*. Harcourt College, NY.
2. Dewick, P.M., (2009). *Medicinal Natural Products: A Biosynthetic Approach*. Wiley and Sons, UK.
3. Finar, I.L. (2006). *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products*. Dorling Kindersley Pvt. Ltd., India.
4. Claydon, J., Gleeves, N., Warren, S. And Wother, P., (2001). *Organic Chemistry*. Oxford University Press, UK.
5. Fleming, I., (2015). *Pericyclic Reactions*. Oxford University Press.
6. Carey B. F. A., and Sundberg R.J., (2007). *Advanced Organic Chemistry Part B*. Springer Science and Business Media Ltd.

**Course Title: Concepts in Chemistry-II****Course Code: CHM.573****Total Contact Hours: 30**

L	T	P	Cr
2	0	0	2

**Learning Outcomes:** The student will be able to

- Know the aspects of structural and bonding of ionic, covalent and coordination molecules and compounds.
- Elucidate the aspects of s, p, d and f-block elements:
- Physical concept involving in quantities errors, Kinetics.
- Thermodynamics, photochemistry and electrochemistry.

**Unit I****7 Hours**

**Structure and bonding:** Electronic configuration of atoms (L-S coupling) and the periodic properties of elements; Ionic radii, Ionisation potential, electron affinity, electronegativity; concept of hybridisation. Molecular orbitals and electronic configuration of homo- and hetero-nuclear diatomic molecules. Shape of polyatomic molecules; VSEPR theory, Symmetry elements and point groups for simple molecules. Acid and bases concepts, pH and pKa, HSAB concept, Buffer solution. Properties of solid state and solution phase.



**Unit II****8 Hours**

**Aspects of s, p, d and f-block elements:** General characteristics of each block. Chemistry of representative (s and p-block) elements, Coordination chemistry of transition elements. Chemistry of lanthanide and Actinides.

**Unit III****7 Hours**

**Thermodynamics:** Concepts involved in first, second and third law of thermodynamic, Maxwell relations, Helmholtz and Gibbs Energies, equilibrium constant, temperature-dependence of equilibrium constant and Van't Hoff equation, Colligative properties of solutions.

**Unit IV****8 Hours**

**Electrochemistry:** Ionic equilibria, ion conduction mechanism, solutions of nonelectrolytes and electrolytes, electrolytic conductance –Kohlrausch's Law, transport number and its determination, Nernst equation, redox systems, electrochemical cells.

**Basics of Photochemistry:** Absorption, excitation, laws of photochemistry, quantum yield, lifetime of excited states, photochemical stages-primary and secondary process.

**Kinetics:** Introduction, rates of chemical reactions, Kinetics of photochemical reactions.

**Mode of Transactions:** Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brain storming, Tutorial

**Suggested Readings**

1. Cotton, F. A., and Wilkinson, G. (1988). *Advanced Inorganic Chemistry* (Vol. 545). New York: Wiley.
2. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic Chemistry: Principles of Structure and Reactivity*. Pearson Education India.
3. Greenwood, N. N., and Earnshaw, A. (2012). *Chemistry of the Elements*. Elsevier.
4. Miessler, G. L. and Tarr, D. A. (2011) *Inorganic Chemistry*, Pearson Education.
5. Atkins, P. (2010). *Shriver and Atkins' Inorganic Chemistry*. Oxford University Press, USA.
6. Barrow, G. M. (2007) *Physical Chemistry*. Tata McGraw-Hill Publishers.
7. Kapoor, K. L. (2011) *Text Book of Physical Chemistry*. 3/5, Macmillan Publishers.
8. Atkins, P. and De Paula, J. (2009) *Atkins' Physical Chemistry*. Oxford University Press.
9. Moore, J. W. and Pearson, R. G. (1981) *Kinetics and Mechanism*. John Wiley and Sons.
10. Puri, B.R., Sharma L.R. and Pathania, M.S. (2013) *Principles of Physical Chemistry*. Vishal Publishing Company.
11. Laidler, K. J. (1987). *Chemical Kinetics*. Pearson Education Ltd.

12. Rohatgi-Mukherjee, K. K., (1986). *Fundamentals of Photochemistry*. New Age International.

**Course Title: Polymer and Solid State Chemistry**

**Course Code: CHM.571**

**Total Contact Hours: 60**

L	T	P	Cr
3	0	0	3

**Learning Outcome:** After completion of this course, the students will be able to

- Different mechanisms of polymerization, number, weight and viscosity average molecular weights with various techniques
- Processing of thermoplastic and thermosetting polymers, concept of conducting polymers and their applications.
- Physicochemical properties, defects in solid, diffraction techniques, electrical and magnetic properties of materials.

### **Unit I**

**11 Hours**

**Polymers:** Importance of polymers, basic concepts: monomers, repeat Units, degree of polymerization. linear, branched and network polymers, classification of polymers. polymerization: condensation, addition, radical chain-ionic, co-ordination and copolymerization, polymerization conditions and polymer reactions, polymerization in homogeneous and heterogeneous systems.

**Application of Polymers:** Phenol-formaldehyde, urea-formaldehyde, melamine-formaldehyde, epoxy resins and curing agents, polyamides: nylon-6, nylon-6, 6,

### **Unit II**

**11 Hours**

**Polymer Characterization:** Polydispersion-average molecular weight concept, number, weight and viscosity average molecular weights, polydispersity and molecular weight distribution, the practical significance of molecular weight, measurement of molecular weights, light scattering, osmotic and ultracentrifugation methods, analysis and testing of polymers, chemical analysis of polymers, thermal analysis and physical testing-tensile strength.

### **Unit III**

**12 Hours**

**Solid State Structure:** Primitive lattice vectors, reciprocal lattice, crystal systems and symmetry, bravais lattices, lattice energy, crystal structure of diamond, NaCl, KCl, CsCl, TiO<sub>2</sub>, etc,

**Defects:** Intrinsic and extrinsic defects, point, line and plane defects, vacancies, Schottky defects, Frenkel defects, Thermodynamic and structural aspects.

**Diffraction Methods:** Basic concepts of X-ray, electron and neutron diffraction methods, structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase identification, X-ray structure analysis, XRD and its applications, polymorphism and cocrystallization.

**Unit IV****11 Hours**

**Semiconductor and Superconductors:** Band theory, band gap, metals and semiconductors, intrinsic and extrinsic semiconductors, p-n junctions and other applications

**Magnetic Optical Properties:** Classification of magnetic materials, Langevin diamagnetism, magnetic domains and hysteresis, optical reflectance, Raman scattering in crystals, photoconduction, lasers, photovoltaic and photocatalytic effects.

**Nanomaterials:** Nanoparticles: zero dimensional nanostructure, homogeneous and heterogeneous nucleation, metallic nanoparticles- synthesis and applications; nanowires and nanorods: one dimensional nanostructures, spontaneous growth, VLS, electro spinning, lithography; thin film: two dimensional nanostructure- preparation techniques; Langmuir-Blodgett (LB) film growth techniques, photolithography properties and applications.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

**Suggested Readings**

1. Gowariker, V. R., Viswanathan, N. V., and Sreedhar, J. (1986). *Polymer Science*. New Age International.
2. Odian, G. (2004). *Principles of Polymerization*. John Wiley and Sons.
3. Peacock, A. J., and Calhoun, A. (2012). *Polymer Chemistry: Properties and Application*. Carl Hanser Verlag GmbH Co KG.
4. Chandra, R., and Adab, A. (1994). *Rubber and Plastic Waste: Recycling, Reuse and Future Demand*. CDB Publishers.
5. Bahadur, P., and Sastry, N. V. (2005). *Principles of Polymer Science*. Narosa Publishing House, New Delhi.
6. Ashcroft, N. W., and Mermin, N. D. (1976). *Introduction to Solid State Physics*. Saunders.
7. Callister Jr, W. D., and Rethwisch, D. G. (2012). *Fundamentals of Materials Science and Engineering: An Integrated Approach*. John Wiley and Sons.
8. Anderson, J. C., Leaver, K. D., Rawlings, R. D., and Leavers, P. S. (2004). *Materials Science for Engineers*. CRC Press.
9. Keer, H. V. (1993). *Principles of the Solid State*. New Age International.

**Course Title: Advanced Organic Synthesis****Course Code: CHM.574****Total Contact Hours: 60**

L	T	P	Cr
4	0	0	4

**Learning Outcomes:** The students will be able to

- Identify various asymmetric tools for the synthesis of chiral compounds.
- Explore various reagents including organometallic compounds, experimental conditions in organic synthesis.

- Design the synthesis of functionalised molecules utilizing phosphorus and sulphur ylides.

### Unit I

**15 Hours**

**Asymmetric synthesis:** Chiral pools, chiral catalysis: chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. resolution – optical and kinetic, chemo- regio- and stereoselective transformations, organocatalysis and biocatalysis.

### Unit II

**15 Hours**

**Reaction of ylides:** Phosphorus ylide; structure and reactivity, stabilized ylides, effects of ligands on reactivity, Wittig, Wittig-Horner and Wadsworth, Emmons reactions-mechanistic realization; E/Z selectivity for olefin formation, Schlosser modification: Sulphur ylides; stabilized and non-stabilized ylides: thermodynamically and kinetically controlled reactions with carbonyl compounds, regio- and stereo-selective reactions. Nitrogen Ylides, Stevens rearrangement.

### Unit III

**15 Hours**

**Organometallic compounds:** Organoboranes: Preparation of organoboranes viz hydroboration with  $\text{BH}_3\text{-THF}$ , dicyclohexyl borane, disiamylborane, tetrabutylborane, 9-BBN, diisopinocampheyl borane, Metal catalysed hydroboration, functional group transformations of organo boranes: oxidation, protonolysis and rearrangements. formation of carbon-carbon-bonds viz organoboranes carbonylation.

Organolithium, organozinc, organosilicon, organopalladium and organostannous compounds: applications in C-C coupling reactions.

### Unit IV

**15 Hours**

**Reagents in organic synthesis:** Gilman's reagent, Lithium diisopropylamide(LDA), 1,3-Dithiane (Umpolungreagent), Trimethylsilyl iodide, Baker's yeast, Prevost Hydroxylation, Crown ether, Merrifield resin, Fenton's reagents, Ziegler-Natta catalyst, Lawesson reagents, IBX, Fetizon reagent, Dioxiranes, Tebbe reagent, Corey-Nicolaou reagent and macrolactonisation, Mosher's reagent.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

### Suggested Readings

1. Mundy, B. P., Ellerd, M. G., and Favalaro Jr, F. G., (2005). *Name Reactions And Reagents In Organic Synthesis*. John Wiley and Sons.
2. Claydon, J., Gleaves, N., Warren, S., and Wother, P., (2001). *Organic Chemistry*. Oxford University Press, UK.
3. Finar, I.L., (2012). *Organic Chemistry*. Pearson Education, UK.

- Li, J. J., (2014). *Name Reactions: A Collection of Detailed Reaction Mechanism*. Springer-Verlag.
- Smith, M. B., (2013). *March's Advanced Organic Chemistry: Reactions, Mechanisms, And Structure*. John Wiley and Sons.
- Corey, E.J. and Cheng, X.-M.(1989). *The Logic of Chemical Synthesis*. John Wiley and Sons.
- Fuhrhop, J. H., Penzlin, G., and Li, G., (2003). *Organic Synthesis: Concepts And Methods*. John Wiley and Sons.
- Davies, S. G., (2013). *Organotransition Metal Chemistry: Applications to Organic Synthesis: Applications to Organic Synthesis* (Vol. 2). Elsevier.
- Aitken, A., and Kilényi, S. N., (Eds.). (1992). *Asymmetric Synthesis*. CRC Press.
- Proctor G. (1996). *Asymmetric Synthesis*. Academic Press.

**Course Title: Chemistry of Natural Products**

**Course Code: CHM.575**

L	T	P	Cr
4	0	0	4

**Total Contact Hours: 60**

**Learning Outcome:** At the end of this course student will be able to

- Recognize various types of natural products and their importance.
- Identify various types of natural products including their properties, occurrence, structure and biosynthesis.

**Unit I**

**15 Hours**

**Terpenoids and Carotenoids:** Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Geraniol, Menthol and  $\beta$ -Carotene

**Unit II**

**15 Hours**

**Alkaloids:** Nomenclature and physiological action, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, structure, stereochemistry, synthesis of the following: Ephedrine, Nicotine and Morphine.

**Unit III**

**15 Hours**

**Steroids:** Occurrence, nomenclature, basic skeleton and stereochemistry, structure determination and synthesis of cholesterol, partial synthesis of testosterone and progesterone, chemical tests for steroids

**Unit IV****15 Hours**

**Plant pigments:** Occurrence, nomenclature and general methods of structure determination. isolation and synthesis of anthocyanins

**Carbohydrates:** Introduction of sugars, structures of triose, tetrose, pentose, hexose, stereochemistry and reactions of glucose, conformation and anomeric effects in hexoses

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

**Suggested Readings**

1. Bhat, S.V., Nagasampagi, B.A., and Meenakshi, S. (2009). *Natural Product Chemistry and Applications*. Narosa Publishing House, New Delhi.
2. Bhat, S.V., Nagasampagi, B.A., and Sivakumar, M. (2005). *Chemistry of Natural Products*. Narosa Publishing House, New Delhi.
3. Cseke, L.J., (2009). *Natural Products from Plants*. CRC Press.
4. Dewick, P.M. (2009). *Medicinal Natural Products: A Biosynthetic Approach*. Wiley and Sons, UK.
5. Finar, I.L., (2006). *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products*. Dorling Kindersley Pvt. Ltd., India.
6. Peterson, F. and Amstutz, R., (2008). *Natural Compounds as Drugs*. Birkhauser-Verlay.

**Course Title: Organotransition Metal Chemistry**

**Course Code: CHM.576**

**Total Contact Hours: 60**

L	T	P	Cr
4	0	0	4

**Learning Outcome:** At the end of this course student will be able to

- The chemistry of transition metal complexes and compounds of transition metal-carbon multiple bonds
- Chemistry on alkyls and aryls of transition metals and fluxional organometallic compounds
- Workout on homogeneous catalysis with appropriate planning.

**Unit I****15 Hours**

**Compounds of Transition Metal-Carbon Multiple Bonds:** Metal Carbenes (Alkylidenes) and carbynes (alkylidynes) complex-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reaction on the ligands, role in organic synthesis

**Unit II****15 Hours**

**Transition Metal Complexes:** Transition metal complexes with alkyl and unsaturated organic molecules, alkenes, alkynes, allyl, diene, dienyl, arene and

trienyl complexes, preparations, properties, nature of bonding and structural features important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis.

### Unit III

**15 Hours**

**Aryls of Transition Metals:** Types, routes of synthesis, stability and decomposition pathways, applications in organic synthesis.

### Unit IV

**15 Hours**

**Homogeneous Catalysis:** Stoichiometric reaction for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction) oxo-palladation reactions, activation of C-H bond.

**Mode of Transactions:** Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brain storming, Tutorial.

### Suggested Readings

1. Collman, J.P., Norton, J.R., Hegsdus, L.S. and Finke, R.G., (1987) *Principles and Application of Organotransition Metal Chemistry*. University Science Books.
2. Crabtree, R.G. (2011). *The Organometallic Chemistry of the Transition Metals*. John Wiley.
3. Mehrotra, R. C., and Singh, A., (2005). *Organometallic Chemistry*. New Age International.
4. Cotton, F.A., and Wilkinson, G., (1999). *Advanced Inorganic Chemistry*. John Wiley.
5. Pearson, A.J., (1985). *Metallo-Organic Chemistry*. Wiley.

**Course Title: Environmental Chemistry**

**Course Code: CHM.577**

**Total Lectures: 60**

L	T	P	Cr
4	0	0	4

**Learning Outcome:** The student will be able to

- Know the various chemical processes in the air water and soil environment
- Apply various policy implication for applied chemists
- Become expertise for treatment technologies adopted for various wastewaters

### Unit I

**15 Hours**

**Aquatic chemistry:** Surface, ground water, marine and brackish water resources - assessment and utilization; Rivers and Lakes in India; hydrological cycle; Structure and properties of water, Water quality parameters,

Physicochemical concepts of color, odour, turbidity, pH, conductivity, DO, COD, BOD and its kinetics, Carbonates and alkalinity, redox potential, Pourbiax diagram, pH-pE diagrams for Iron, oxoanions and anions, Environmental Issues: Ground water depletion; Water logging and salinity; Water Conservation and management techniques; Rain water harvesting; Watershed management; Eutrophication; Restoration of Lakes, transboundary river water sharing and interlinking of rivers.

**Interfacial Interactions:** Environmental chemistry of arsenic, chromium, Chemical potential, fugacity and its application to fugacity model.

## **Unit II**

**15 Hours**

**Water treatment Technologies:** Chemical and Physical Methods of wastewater treatment with emphasis on sedimentation, coagulation, adsorption, water softening, defluoridation and ion exchange process.

**Membrane Processes:** Reverse Osmosis, Types of membrane, characterization of membranes, nano-membranes and their formation, efficiency of different membranes in removal of different elements.

**Biological wastewater treatment** including Activated sludge process, trickling filter and Membrane bioreactor, biological treatment processes - process description, design and application.

## **Unit III**

**15 Hours**

**Atmospheric chemistry:** Composition of air, Chemical speciation, particles, ion and radicals, Formation of particulate matter, Photochemical reactions in the atmosphere, Chemistry of air pollutants, Photochemical smog, Acid rain, Ozone Chemistry and Montreal Protocol, Greenhouse gases and Global warming, Clean Development Mechanism and Kyoto Protocol, Persistent Organic Pollutants (POP) and Stockholm Convention.

**Sources of Natural and Artificial Radiations:** Dosimetry, types of dosimeters, radioactive substances, applications and handling of isotopes and other radionuclides in environment. Biochemical and Toxicological aspects of arsenic, cadmium, lead, mercury, carbon monoxide, O<sub>3</sub>, PAN, MIC and other carcinogens.

## **Unit IV**

**15 Hours**

**Chemistry of Soil:** Physio-chemical composition of soil, humus, inorganic and organic components of soil, nutrients (NPK) in soil, significance of C:N ratio, cation exchange capacity (CEC), reactions in soil solution, ion exchange (physiosorption), ligand exchange (chemisorption), complexations, chelation; precipitation / dissolution.

**Environmental Geochemistry:** Concept of major, trace and REE. classification of trace elements, mobility of trace elements, geochemical cycles.

**Waste Management:** Biomass waste management, biomedical waste management and chemical waste management, design and construction of waste management site. Regulations for waste management.



**Mode of Transactions:** Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brain storming, Tutorial

**Suggested Readings**

1. Baird, C., and Cann, M., (2008). *Environmental Chemistry*. W.H. Freeman, USA
2. Manahan, S. E., (2008). *Fundamentals of Environmental Chemistry*. CRC Press, USA
3. Connell D. W. (2005). *Basic concepts of Environmental Chemistry*, CRC Press, USA
4. Girard, J., (2010). *Principles of Environmental Chemistry*. Barlett Publishers, USA.
5. Harrison, R. M., (2007). *Principles of Environmental Chemistry*. RSC Publishing, UK
6. Hillel, D., (2007). *Soil in the Environment: Crucible of Terrestrial Life*. Academic Press, USA.
7. Manahan, S. E., (2010). *Water Chemistry: Green Science and Technology of Natures Most Renewable Resource*. CRC Press, USA.
8. Tchobanoglous, G., Burton, F. L., and Stensel, H. D., (2003). *Wastewater Engineering: Treatment and Reuse*. McGraw-Hill Science, USA.
9. American Public Health Association, American Water Works Association and Water Environment Federation, (2005). *Standard Methods for the Examination of Water and Wastewater*. American Public Health Association.
10. Eckenfelder, Jr., W.W., Ford, D.L., and Englands, A.J., Jr. (2009). *Industrial water quality*. McGraw-Hill.
11. Crittenden, J. C., Trussell, R. R., and Hand, D. W., (2005). *Water treatment: principles and design*. Wiley Publishers, USA.
12. Grady Jr, C. L., Daigger, G. T., Love, N. G., and Filipe, C. D. (2011). *Biological Wastewater Treatment*. CRC Press.

**Course Title: Inorganic Photochemistry**

**Course Code: CHM.578**

**Total Contact Hours: 60**

L	T	P	Cr
4	0	0	4

**Learning Outcomes:** The student will be able to

- Inorganic photochemistry and photophysical chemistry.
- The characterization of transient intermediates by ultrafast modern techniques.
- The theory of photoreaction.
- The photochemistry and photophysical chemistry of macromolecules.

**Unit I**

**15 Hours**

**Basics of Photochemistry:** Electronic transitions, Jablonski diagram and photophysical processes, radiative transitions, absorption and emission,

phosphorescence, intersystem crossing, mechanisms of singlet-triplet conversion (spin-orbit coupling), examples of ISC between states of different configurations, radiative rates, radiationless transitions, internal conversion, energy gap.

## **Unit II**

**15 Hours**

**Photochemical Mechanism:** Properties of excited states- structure, dipole moment, photochemical kinetics- calculation of rates of radiative process; bimolecular deactivation- quenching; excited states of metal complexes comparison with organic compounds, electronically excited states of metal complexes, charge transfer excitation.

## **Unit III**

**15 Hours**

**Ligand Field Photochemistry:** Photosubstitution, photooxidation and photoreduction, ground state and excited state, energy content of the excited state, development of redox potentials of the excited states; redox reactions by excited metal complexes- energy transfer(FRET and SET), exciplex formation,

## **Unit IV**

**15 Hours**

**Applications of Photochemistry:** Measurement of fluorescence and phosphorescence and lifetimes, introduction to time-resolved techniques for absorption and emission measurements, detection and kinetics of reactive intermediates, photochromic reactions and memory devices, sensors, switches and molecular machines, TiO<sub>2</sub> photocatalysis, flash photolysis.

**Mode of Transactions:** Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brain storming, Tutorial

### **Suggested Readings**

1. Lakowicz, J. R., (2006). *Principles of Fluorescence Spectroscopy*, Springer.
2. Rohatgi-Mukherjee, K. K., (1986). *Fundamentals of Photochemistry*. New Age International.
3. Kryukov, A. I., and Yakuchmii, S., (1990). *Fundamentals of Photochemistry of Coordination Compounds*.
4. Kavarnos, G. J. (1993). *Fundamentals of Photoinduced Electron Transfer*. Vch Pub.
5. Valeur, B., andBerberan-Santos, M. N. (2012). *Molecular Fluorescence: Principles and Applications*. John Wiley and Sons.
6. Turro, N. J., Ramamurthy, V., andScaiano, J. C. (2012). *Modern Molecular Photochemistry of Organic Molecules*. Wiley Publishers.
7. Ninomiya, I., and Naito, T. (2012). *Photochemical Synthesis*. Academic Press.

**Course Title: Supramolecular Chemistry**

**Course Code: CHM.580**

**Total Contact Hours: 60**

L	T	P	Cr
4	0	0	4

**Learning Outcome:** The students will acquire knowledge of

- Various supramolecular aspects of interaction between two chemical systems.
- Devising supramolecular systems based on complementarily and preorganizational requirements of host.

### **Unit I**

**15 Hours**

**Introduction:** Definition and development of supramolecular chemistry, nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, h-bonding, cation- $\pi$ , anion- $\pi$  and van der waals interactions, supramolecular chemistry in life, ionophores, porphyrin and other tetrapyrrolic macrocycles, coenzymes, neurotransmitters, DNA and biochemical self-assembly. Classification of supramolecular host-guest compounds, pre-organization and complementarily, receptors, nature of supramolecular interactions.

Host-guest chemistry: synthesis and structure of crown ethers, lariat ether and podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, carcerands and hemicarcerands. Concepts of selectivity, macrocyclic, macrobicyclic synthesis and template effects,

### **Unit II**

**15 Hours**

**Cation Binding:** Binding Constant and its determination, concept of coordination chemistry, cation complexation using various preorganized host, soft ligands including N, S and P based macrocycles, Schiff's base, proton and ammonium ion complexation, carbon donor and  $\pi$ -acid ligands, siderophores.

**Anion Receptor:** Anion recognition and its biological relevance, concepts on anion host design, from cation to anion hosts- a simple change in pH, guanidinium-based receptors, neutral receptors, organometallic receptors, coordination interactions. Chromogenic and fluorogenic receptors, dosimeters, ion pair recognition and zwitterion recognition.

**Inclusion Complexes:** Molecular guests and their inclusion complexation with Cyclodextrin, molecular clefts, tweezers, cryptophanes, cyclophanes, carcerands and hemicarcerands, solid state inclusion including clathrate formation, solid-liquid, solid-gas inclusions.

### **Unit III**

**15 Hours**

**Molecular Self-assembly:** Supramolecular polymers: definition, kinetic and thermodynamic consideration of self-assembly. self-assembly molecules: design, synthesis and properties of the molecules, self-assembly by H-bonding, proteins and foldamers, DNA, catenanes, rotaxanes, molecular knot: topology and

examples including trefoil and borromean rings, surfactants self assembly, liquid crystals.

Dendrimers structure and nomenclature, synthesis and characterization, supramolecular chemistry of dendrimers and its assembly, dendritic nanodevices  
Supramolecular polymers including amphiphilic block polymers and molecular imprinter polymers, biological self assembly in amyloids, actins and fibrin, COF and supramolecular gels.

#### **Unit IV**

**15 Hours**

**Supramolecular and Molecular Devices:** Supramolecular photochemistry and catalysis, molecular electronic devices: molecular electronic devices, molecular wires, molecular rectifiers, molecular switches and molecular logic gates, non linear optical devices, organics for photonics and electronics.

**Molecular Machines:** Molecular machine terminology and bio-inspiration, ratchet mechanism including pulsating and tilt mechanism, covalent and supramolecular motors and their controlling mechanisms, machines based on catenanes and rotaxanes. Applications as molecular walkers, switchable catalysts, surface analysis at molecular dimensions.

**Mode of Transactions:** Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brain storming, Tutorial

#### **Suggested Readings**

1. Steed, J. W., and Atwood, J. L. (2013). *Supramolecular chemistry*. John Wiley and Sons.
2. Lehn, J. M., (1995). *Supramolecular Chemistry-Concepts and Perspectives*. Wiley –VCH.
3. Beer, P.D., Gale, P. A., and Smith, D. K., (1999). *Supramolecular Chemistry*. Oxford University Press.
4. Martin, N. and Nierengarten J.-F. (2012). *Supramolecular Chemistry of Fullerenes and Carbon Nanotubes*. Wiley-VCH.
5. Vicens, J. and Harrowfield J. (2007). *Calixarenes in the Nanoworld*. Springer.
6. Schalley, C. A. (2012). *Analytical Methods in Supramolecular Chemistry*. Vol. 1 and 2, Wiley-VCH.
7. Erbas-Cakmak, S., Leigh, D. A., McTernan, C. T., and Nussbaumer, A. L. (2015). Artificial molecular machines. *Chemical Review*, 115(18), 10081-10206.

**Course Title: Material Chemistry**

**Course Code: CHM.581**

**Total Contact Hours: 60**

L	T	P	Cr
3	0	0	4

**Learning Outcome:** The students will be able to learn

- Inorganic, organic and mixed materials
- Characterization of these materials
- The relationship between material structure and physical attributes associated with them.

### **Unit I**

**15 Hours**

**Magnetic Materials (Ferrites)** Introduction, structure and classification, hard and soft ferrites, synthesis of ferrites by various methods (precursor and combustion method), characterization of ferrites by Mossbauer spectroscopy, significance of hysteresis loop and saturation magnetization in ferrites, magnetic properties of ferrites, applications of ferrites.

**Glasses, Ceramics, Composites and Nanomaterials:** Glassy state, glass formers and glass modifiers, applications. ceramic structures, mechanical properties, clay products. microscopic composites; dispersion-strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites, nanocrystalline phase, preparation procedures, special properties, applications.

### **Unit II**

**15 Hours**

Mesomorphic behaviour, thermotropic liquid crystals, positional order, bondorientational order, nematic and smectic mesophases; smectic - nematic transition and clearing temperature -homeotropic, planar and sCHMieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic A and smectic C phases, optical properties of liquid crystals. dielectric susceptibility and dielectric constants. lyotropic phases and their description of ordering in liquid crystals.

#### **Thin Films and Langmuir- Blodgett Films**

Preparation techniques; evaporation/sputtering, chemical process, sol gel etc. Langmuir – Blodgett (LB) films, growth technique, photolithography, properties and applications of thin and LB films

#### **Materials for Solid State Devices**

Rectifiers, transistors, capacitors –IV-V compounds, low-dimensional quantum structure; optical properties.

### **Unit III**

**15 Hours**

Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors; phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.

**Molecular Conductor:** Oligo(phenylenevinylene)s, oligo(phenyleneethynylene)s, oligo(ene-yne)s, oligo(thiophenevinylene), oligo(thiopheneethynylene) etc. and their applications.

**Preparation and characterization of silica and zirconia based stationary phases** by (a) dynamic chemical modification, in which chiral selector is adsorbed on the surface of the zirconia by physical forces, (b) permanent chemical modification, in which a CS is chemically bonded onto the zirconia surface, and (c) physical screening, in which zirconia surface is coated with a polymer or carbon layer, and their application in chiral separations by LC

#### Unit IV

15 Hours

**Fullerenes, Carbon Nanotubes and Graphene:** Types and Properties, methods of preparation and separation of carbon nanotubes, applications of fullerenes, CNTs and graphene.

**Nonlinear optical materials:** Non-linear optical effects, second and third order – molecular hyperpolarisability and second order electric susceptibility – materials for second and third harmonic generation.

**Mode of Transactions:** Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brain storming, Tutorial

#### Suggested Readings

1. Ashcroft, N. W., and Mermin, N. D. (1976). *Introduction to Solid State Physics*. Saunders.
2. Callister Jr, W. D., and Rethwisch, D. G. (2012). *Fundamentals of Materials Science and Engineering: An Integrated Approach*. John Wiley and Sons.
3. Anderson, J. C., Leaver, K. D., Rawlings, R. D., and Leever, P. S. (2004). *Materials Science for Engineers*. CRC Press.
4. Keer, H. V. (1993). *Principles of the Solid State*. New Age International.

**Course Title: Project**

**Course Code: CHM.599**

**Total Contact Hours: 180**

L	T	P	Cr
0	0	0	6

**Learning Outcome:** The student would be able to

- Investigate various aspects related to the chemistry problem.
- Appreciate the literature and its relevance to his topic of interest
- Write research proposal independently
- Would generate interest in current topics of research.

Project supervisor would be allocated at the start of the semester and research project would be undertaken in discussion with the project supervisor. At the end of the semester the student has to prepare a project report as per the university guidelines. Upon submission of the project report, the projects would be evaluated based on a project presentation.

**Course Title: Basic Perspectives in Inorganic Chemistry****Course Code: CHM.515****Total Contact Hours: 30**

L	T	P	Cr
2	0	0	2

**Learning Outcome:** The student will be able to

- Become expert in the coordination chemistry of d-group elements and coordination of ions within living organisms.
- Know the environmental chemistry and metal hydrides as hydrogen energy source.

**Unit I****7 Hours**

Chemistry of d-block elements, coordination chemistry, models and stereochemistry, theories, spectra and bonding.

**Unit II****8 Hours**

**Ions role in bioscience:** ionophores, porphyrin and other tetrapyrrolic macromolecules, coenzymes, neurotransmitters, metal binding to DNA.

**Unit III****8 Hours**

**Metals in aqueous environment:** Introduction, environmental chemistry, environmental composition, chemical processes, complexes, metal speciation of calcium, copper and mercury, their behaviour in hydrosphere.

**Unit IV****7 Hours**

**Hydrogen Energy:** introduction, synthesis and structures of metal hydrides, coordination modes of hydrogen atom, hydrogen storage, H<sub>2</sub> evolution under solar energy, thermal energy and acidifications.

**Mode of Transactions:** Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brain storming, Tutorial

**Suggested Readings**

1. Lippard, S.J. and Berg, J.M., (1994) *Principles of Bioinorganic Chemistry*. University Science Books.
2. Cotton, F. A., and Wilkinson, G. (1988). *Advanced Inorganic Chemistry* (Vol. 545). New York: Wiley.
3. Huheey, J. E., Keiter, E. A., Keiter, R. L., and Medhi, O. K. (2006). *Inorganic Chemistry: Principles of Structure and Reactivity*. Pearson Education India.
4. Greenwood, N. N., and Earnshaw, A. (2012). *Chemistry of the Elements*. Elsevier.
5. Van-Loon G.W. and Duffy S.J. (2011) *Environmental Chemistry: A Global Perspective*. Oxford University Press.
6. Rao C.S. (2006) *Environmental Pollution Control Engineering*. New Age International Publishers, New Delhi,
7. Peruzzini, M. and Poli, R. (2005) *Recent Advances in Hydride Chemistry*, Elsevier Science B.V., Amsterdam.

**Course Title: Introduction to Green Chemistry and Sustainability**

**Course Code: CHM.516**

**Total Contact Hours: 30**

L	T	P	Cr
2	0	0	2

**Learning objective:** Students will be able to

- Know the concept and various tools of Green Chemistry.
- Explain the relevance of Green Chemistry in the context of environment issues.
- Realise the judicious utilization of abundantly available precursors instead of depleting petroleum based feedstocks.

**Unit I**

**7 Hours**

**Introduction:** Adverse effect of some of the current chemical practices on health and environment, concept and need of green chemistry, basic principles of green chemistry with examples– atom economy, wastage minimization, selection of starting materials etc. limitations/obstacle in the pursuit of the goals of green chemistry, types of solvent.

**Unit II**

**7 Hours**

**Emerging non-conventional techniques:** Microwave heating as energy efficient source, mechanism of microwave heating, Examples of microwave assisted organic synthesis, sono-chemistry and green chemistry,

**Unit III**

**8 Hours**

**Green solvents:** Ionic liquids: properties and advantages, use of ionic liquids as solvent as well as catalyst, recyclability of ionic liquids. Solvent-free synthesis.

**Unit IV**

**8 Hours**

**Value addition of abundantly available precursors:** Need for the use of renewable precursors over petroleum based feedstocks, biomass conversion (carbohydrates, lignocellulose biomass) into value added molecules.

**Mode of Transactions:** Lecture, Demonstration, Presentation, Group Discussion, Lecture cum demonstration, Problem solving, Brain storming

**Suggested Readings**

1. Anastas, P.T. and Warner J. C. (2000) *Green chemistry: Theory and Practical*. Oxford University Press, US.
2. Ahluwalia, V.K and Kidwai, M. (2004) *New Trends in Green Chemistry*. Springer.
3. Malhotra, S. V. (2007) *Ionic Liquids in Organic Synthesis*. Oxford University Press, US.
4. Ahluwalia, V.K. (2011) *Green Chemistry: Greener Alternatives to Synthetic Organic Transformations*. Alpha Science International Limited.



5. Klass, D. (1998) *Biomass for Renewable Energy, Fuels, and Chemicals*. Elsevier.

**Course Title: Chemicals of Everyday life**

**Course Code: CHM 519**

**Total Lectures: 36**

L	T	P	Cr
2	0	0	2

**Learning objective:** Students will be able to

- Know the utility of various chemical in daily routine life.
- Explain the importance of green approaches as the need of the hour

### **Unit I**

**5 Hrs**

#### **Chemicals and safety**

Chemicals in daily life, Cosmetics, Perfumes, Soaps and detergents, Cleaning action of detergent, Handling of strong acids and bases, Disinfectant, Insecticides and pesticides, Chemical treatment of vegetables and fruits

### **Unit II**

**5 Hrs**

#### **Common chemical processes**

Chemical reactions, Basics of organic synthesis, Chemistry of photosynthesis, Rusting, Electrochemical cells, Metal electroplating, Acid base titration in the lab Use of polymers in daily life, Polymer based products, Teflon, Polystyrene, Plastic bags, ATM cards.

### **Unit III**

**10 Hrs**

#### **Chemistry of small bioactive molecules**

Caffeine, Nicotine, Paracetamol, Aspirin, DNA and RNA bases, Carbohydrates Abused substances like morphine, Cannabis, Cocaine etc.

### **Unit IV**

**10 Hrs**

#### **Green chemical processes**

Environment friendly process, Principle of green chemistry, Atom economy and scope, Prevention/Minimization of hazardous/toxic products, Designing safer chemicals, Selection of appropriate auxiliary substances (solvents, separation agents etc), Use of renewable starting materials, Avoidance of unnecessary derivatization-careful use of blocking/protection groups

**Microwave in organic synthesis:** Introduction to synthetic organic transformation under microwave (i) Microwave assisted reactions in water (ii) Microwave assisted reactions in organic solvents. (iii) Microwave in solvent free reactions.

**Mode of Transactions:** Lecture, Demonstration, Lecture cum demonstration, Problem solving, Brain storming, Tutorial.

### Suggested Readings

1. Singh, K.; *Chemistry in Daily Life*, PHI learning, 3<sup>rd</sup> edition India
2. Glasstone, S.; *Chemistry in Daily Life*, Cornell University, Methuen & Company Limited, 1929
3. Cohan, L.; *Chemistry in Daily Life; Popular Lectures*, HardPress, 2012
4. Anastas, P.T.; Warner J. C. (2000). *Green chemistry, Theory and Practical*. Oxford University Press, 1<sup>st</sup> edition, US.
5. Grieco, P.A. (1997). *Organic Synthesis in Water*. Blackie, 1<sup>st</sup> edition

**Course Title: Chemistry of Nanomaterials and Fabrication**  
**Course Code: CHM.517**

**Total Contact Hours: 30**

L	T	P	Cr
2	0	0	2

**Learning Outcome:** The students will acquire knowledge of Nanotechnology, fabrication and characterization of nanomaterials, properties and applications of nanomaterials.

### Unit I

**7 Hours**

#### Background to Nanotechnology:

Scientific revolution- Atomic structures-molecular and atomic size-Bohr radius -emergence of nanotechnology-challenges in nanotechnology.definition of a nano system - types of nanocrystals-one dimensional (1D)-two dimensional (2D)-three dimensional(3D) nanostructured materials - quantum dots - quantum wire-multifunctional nanostructures.

### Unit II

**7 Hours**

**Fabrication and Characterization of Nanomaterials:** Top-down and bottom-up approaches: chemical routes for synthesis of nanomaterials: chemical precipitation and coprecipitation; metal nanocrystals by reduction, sol-gel synthesis; microemulsions or reverse micelles, myle formation; solvothermal synthesis; thermolysis routes, microwave heating synthesis; sonochemical synthesis; electrochemical synthesis. physical methods: -inert gas condensation, arc discharge, plasma arc technique, MW plasma, laser pyrolysis, molecular beam epitaxy, chemical vapour deposition method and electro deposition. diffraction analyses, imaging techniques, spectroscopic techniques.

### Unit III

**8 Hours**

**Nanomaterials and properties:**Influence of nucleation rate on the size of the crystals- macroscopic to microscopic crystals andnanocrystals - large surface to volume ratio. Metals (Au, Ag) - metal oxides (TiO<sub>2</sub>, CeO<sub>2</sub>, ZnOetc) - semiconductors (Si, Ge, CdS, ZnSe) - carbon nanotubes (CNT) - ceramics and composites - dilute magnetic semiconductor- biological system - DNA and RNA -

lipids - size dependent properties - mechanical, physical and chemical properties.

#### Unit IV

**8 Hours**

**Applications of Nanomaterials:** Photocatalysis- solar cell-water splitting-energy harvesting- LSPR- molecular electronics and nanoelectronics- quantum electronic devices - CNT based transistor and field emission display -biological applications - biochemical sensor-MRI agent - nanomedicine: molecular manufacturing - MEMS - NEMS - Bio-MEMS - protein nanoarrays - nano fluidics and micro fluidics -self-assembly of nanoparticles for biomedical applications-bacterial structures- cubosomes-dendrimers-DNA nanoparticle conjugates-bioactive nanomaterials-Au nanoparticles and CdSe quantum dots - molecular motors -nanoparticle and protein interactions.

#### Suggested Readings

1. Rao, C. N. R., Müller, A. and Cheetham, A. K. (Eds.) (2004). *The Chemistry of Nanomaterials: Synthesis, Properties and Applications*. Willy-VCH.
2. Poole, Jr., C. P. and Owens F. J. (2006). *Introduction to Nanotechnology*, Willy-VCH
3. Mukhopadhyay, S. M., (2012) *Nanoscale Multifunctional Materials: Science and Applications*. Willy-VCH
4. Kelsall, R. W., Hamley, I. W. and Geoghegan, M. (2005). *Nanoscale Science and Technology*. 2005, John Wiley and Sons.

**Course Title: General Laboratory Practice**

**Course Code: CHM.518**

L	T	P	Cr
2	0	0	2

**Total Contact Hours: 30**

**Learning Outcome:** The students will acquire knowledge of

- Good laboratory practices
- Quality control and Quality assurance
- Chemical, biological and radiational hazards in laboratory and safety.
- General know how of analytical sample preparation.

#### Unit I

**7 Hours**

**Good Laboratory Practices:** Introduction and WHO guidelines on GLP and GMP. History of GLP. Quality assurance in GLP. Quality control laboratory, responsibilities, routine controls, instruments reagents, sampling plans.

#### Unit II

**8 Hours**

**Quality Standards and Quality Assurances:** Advantages and disadvantages of quality standards, concepts of quality control, quality assurance its functions and advantages. Standard test procedures, protocols, non-clinical testing,

controls on animal house, data generation and storage, quality control documentation, retention samples, records. Complaints and recalls, evaluation of complaints, recall procedures, related records and documents.

### **Unit III**

**8 Hours**

**Safety and Hazard Analysis:** Chemical classification of hazards, Radiation hazard, AERB regulation for Fire and its prevention, biosafety and biohazard. Weapons of Mass destruction

### **Unit IV**

**7 Hours**

**Basic Analytical practices:** Titrimetry, Gravimetric analysis, Potentiometry and Spectrophotometric analysis. Pesticides and pesticide residue extraction, Solid phase extraction etc. Trace metal sample preparations and analysis. Proteomic and metabolomic sample preparations

### **Suggested Readings**

1. Miller, J. C. Miller, J. N. (1998) *Statistics for Analytical Chemistry*. Wiley.
2. [http://www.who.int/water\\_sanitation\\_health/resourcesquality/wqmchap9.pdf](http://www.who.int/water_sanitation_health/resourcesquality/wqmchap9.pdf)
3. <https://www.unece.org/fileadmin/DAM/env/water/publications/documents/guidancelaboratories.pdf>.

IQAC