

# **Course Structure and Syllabus**

**M.Sc. Chemistry (CBCS)**

**(SEMESTER: I - IV)**

**(FOR NEW ADMISSION)**

**Examinations: 2016-17**

**Centre for Chemical Sciences  
School of Basic and Applied Sciences  
Central University of Punjab  
Mansa Road  
Bathinda – 151001**

**Centre for Chemical Sciences  
M.Sc. Chemistry**

**SEMESTER 1**

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	Weightage (%)				E
								A	B	C	D	
1	CHL.501	Chemical Biology (Non-medical group)	FC	2	-	-	2	10	15	15	10	50
	CHL502	Chemical Mathematics (Medical group)										
3	CHL.503	Analytical Chemistry and Instrumental Methods	CC	4	1	-	4	25	25	25	25	100
4	CHL.504	Inorganic Chemistry-1	CC	4	1	-	4	25	25	25	25	100
5	CHL.506	Organic Chemistry-I	CC	4	1	-	4	25	25	25	25	100
6	CHL.508	Physical Chemistry-I	CC	4	1	-	4	25	25	25	25	100
7	CHP.505	Practical Inorganic Chemistry-1	CC	-	-	4	2	-	-	-	-	50
8	CHP.507	Practical Organic Chemistry-I	CC	-	-	4	2	-	-	-	-	50
9	XXX	Inter-Disciplinary Course (ID)  (Opt any one from other Departments)	EC	2	-	-	2	10	15	15	10	50
<b>Total</b>				<b>20</b>	<b>4</b>	<b>8</b>	<b>24</b>					<b>600</b>

**FC:** Foundation Course, **CC:** Core Course, **EC:** Elective Course

**A:** Surprise Tests (minimum three): Based on Objective Type Tests

**B:** Mid-Semester Test – I: Based on Subjective Type Test

**C:** Mid-Semester Test – II: Based on Subjective Type Test

**D:** End-Term Exam (Final): Online Objective Type Test

**E:** Total Marks

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

## SEMESTER 2

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	Weightage (%)				E
								A	B	C	D	
1	CHL.521	Inorganic Chemistry-II	CC	4	1	-	4	25	25	25	25	100
2	CHL.523	Organic Chemistry-II	CC	4	1	-	4	25	25	25	25	100
3	CHL.524	Physical Chemistry-II	CC	4	1	-	4	25	25	25	25	100
4	CHL.526	Quantum Chemistry	CC	4	1	-	4	25	25	25	25	100
5	CHP.522	Practical Inorganic Chemistry-II	CC	-	-	4	2	-	-	-	-	50
6	CHP.525	Practical Physical Chemistry- II	CC	-	-	4	2	-	-	-	-	50
7	CHS.599	Seminar	EC	-	-	-	2	-	-	-	-	50
8	XXX	Inter-Disciplinary Course (ID) (Opt any one from other Departments)	EC	2	-	-	2	10	15	15	10	50
<b>Total</b>				<b>18</b>	<b>4</b>	<b>8</b>	<b>24</b>					<b>600</b>

**FC:** Foundation Course, **CC:** Core Course, **EC:** Elective Course

**A:** Surprise Tests (minimum three): Based on Objective Type Tests

**B:** Mid-Semester Test – I: Based on Subjective Type Test

**C:** Mid-Semester Test – II: Based on Subjective Type Test

**D:** End-Term Exam (Final): Online Objective Type Test

**E:** Total Marks

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

### SEMESTER 3

S. No.	Paper Code	Course Title		L	T	P	Cr	Weightage (%)				E
								A	B	C	D	
1	CHL.601	Inorganic Chemistry-III	CC	4	1	-	4	25	25	25	25	100
2	CHL.602	Organic Chemistry-III	CC	4	1	-	4	25	25	25	25	100
3	CHL.604	Physical Chemistry-III	CC	4	1	-	4	25	25	25	25	100
4	CHL.606	Spectral Analysis	CC	4	1	-	4	25	25	25	25	100
5	CHL.607	Research Methodologies	FC	2	-	-	2	10	15	15	10	50
6.	CHP.603	Practical Organic Chemistry-III	CC	-	-	4	2	-	-	-	-	50
7.	CHS.605	Physical Chemistry-III (Practical)	CC	-	-	4	2	-	-	-	-	50
<b>Opt any one of the following courses:</b>												
8.	CHL.608	Inorganic Photochemistry	EC	4	1	-	4	25	25	25	25	100
	CHL.609	Current trends in Organic synthesis										
	CHL.610	Supramolecular Chemistry										
<b>Total</b>				<b>22</b>	<b>5</b>	<b>8</b>	<b>26</b>					<b>650</b>

**FC:** Foundation Course, **CC:** Core Course, **EC:** Elective Course

A: Surprise Tests (minimum three): Based on Objective Type Tests

B: Mid-Semester Test – I: Based on Subjective Type Test

C: Mid-Semester Test – II: Based on Subjective Type Test

D: End-Term Exam (Final): Online Objective Type Test

E: Total Marks

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

### SEMESTER 4

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	Weightage (%)				E
								A	B	C	D	
1	CHL.621	Polymer and Solid State Chemistry	CC	4	1	-	4	25	25	25	25	100
<b>Opt any one of the following courses:</b>												
2	CHL.622	Bioinorganic and Biophysical Chemistry	EC	4	1	-	4	25	25	25	25	100
	CHL.623	Advanced Organic Synthesis										
	CHL.624	Material Chemistry										
	CHL.625	Chemistry of Natural Products										
	CHL.626	Organotransition Metal Chemistry										
3	CHD.600	Project	EC	-	-	-	16	-	-	-	-	400
<b>Total</b>				<b>8</b>			<b>24</b>					<b>600</b>

**FC:** Foundation Course, **CC:** Core Course, **EC:** Elective Course

**A:** Surprise Tests (minimum three): Based on Objective Type Tests

**B:** Mid-Semester Test – I: Based on Subjective Type Test

**C:** Mid-Semester Test – II: Based on Subjective Type Test

**D:** End-Term Exam (Final): Online Objective Type Test

**E:** Total Marks

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

L	T	P	Credits	Marks
2	0	0	2	100

**Course Title: Chemical Biology**

**Paper Code: CHL.501**

**Total Lectures: 36**

**Course Objective:** To impart knowledge of molecular structure and interactions present in various biomolecules that assist in functioning and organization of biological cell.

**Unit 1** **9 Hrs**

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

**Unit 2** **9 Hrs**

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

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

**Unit 3** **9 Hrs**

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

Catalysis and binding in enzymes, ligand-protein interactions, membranes, ribosomes and multienzyme complexes as supramolecular complexes.

**Unit 4** **9 Hrs**

**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, genome sequencing and PCR techniques.

**Lipids:** Lipid classification, lipid bilayers, lipoproteins-composition. high density (HDL) and low-density (LDL) lipoproteins and function, membrane proteins - integral membrane proteins, lipid linked proteins, peripheral proteins, overview of membrane structure and assembly, liposomes, their biological functions.

**Course Outcome:**

After this course completion, the students will acquire knowledge of

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

**SUGGESTED READINGS**

1. Voet, D.J., Voet, J.G., Pratt, C.W., Principles of Biochemistry, 3<sup>rd</sup> edition, 2008, John Wiley,.
2. Berg, J.M., and Tymoczko, J.L., Stryer, L., Biochemistry, 6<sup>th</sup> edition, 2007, W.H. Freeman,.

3. Garrett, R.H., Grisham, C.M., Biochemistry, Brooks/Cole, 4<sup>th</sup> edition, 2014, Cengage Learning.
4. Conn, E.E., and Stump, F., Outlines of Biochemistry, 5<sup>th</sup>edition, 2006, John Wiley.

**Course Title: Chemical Mathematics**

**Paper Code: CHL.502**

**Total Lectures: 36**

L	T	P	Credits	Marks
2	0	0	2	100

**Course Objective:** To provide students with knowledge, abilities and insight in mathematics so that they can understand, correlate and quantify the physical principles of chemical system.

**Unit 1** **9 Hrs**

**Trigonometry and Algebra**

Trigonometric functions of sum and differences of angles, addition and subtraction formulas. Quadratic equations and their solutions: binomial theorem, binomial expansion, finding middle term, general term.

**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 2** **9 Hrs**

**Differential Calculus and Matrix Algebra**

Functions, limits, derivative, physical significance, basic rules of differentiation, maxima and minima, exact and inexact differentials, partial differentiation.

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 3** **9 Hrs**

**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 4** **9 Hrs**

**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.

**Course Outcome:**

1. The completion of this course will enable the students to solve the complex problems in quantum chemistry, statistical thermodynamics, molecular spectroscopy, chemical kinetics, group theory, etc in the latter stage of M.Sc. chemistry programme.

**SUGGESTED READINGS**

1. Steiner, E. The Chemistry Mathematics, 2<sup>nd</sup> edition, 2008, Oxford University Press.
2. Doggett, G. and Sucliffe, B.T. Mathematics for Chemistry, 1<sup>st</sup> edition, 1995, Longman.
3. Daniels, F. Mathematical Preparation for Physical Chemistry, 2003, McGraw Hill.
4. Hirst, D.M. Chemical Mathematics, Longman.
5. Barrante, J. R. Applied Mathematics for Physical Chemistry, 3<sup>rd</sup> edition, 2008, PrenticeHall.
6. Tebbutt P. Basic Mathematics for Chemists, 1<sup>st</sup> edition, 1998, John Wiley.



**Course Title: Analytical Chemistry and Instrumental Methods****Paper Code: CHL.503****Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Course Objective:** To impart knowledge of various analytical and instrumental methods for chemical characterization and analysis.

**Unit 1** **18 Hrs**

**Errors in Quantitative Analysis:** Accuracy, precision, sensitivity, specificity, standard deviation, classification of errors and their minimization, significant figures, criteria for rejection of data, Q-test, T-test and F-test, control chart, sampling methods, sampling error, statistical data treatment, standard reference materials, Introduction to chemical metrology.

**Quantitative Analysis:** Concepts important to quantitative analysis, classification of methods for quantitative analysis, choice of method for analysis, Theory of volumetric and gravimetric methods of analysis.

**Unit 2** **18 Hrs**

**Analytical Spectroscopy:** Principle, applications and limitations of spectrophotometry, Beer-Lambert law, analysis of mixtures, sources and treatment of interferences and detection limits to be considered in each of the techniques, fluorescence spectrometry, nephelometry, turbidimetry, atomic absorption spectrometry (AAS); flame AAS, electrothermal AAS (ETAAS). wavelength dispersive (WDXRF) and energy dispersive (EDXRF) X-ray fluorescence

**Mass and Electron Spectroscopy:** Mass spectrometry: mass analysers; magnetic, electrostatic, double focusing, quadrupole, time of flight, ion cyclotron resonance. ion sources, electron impact ionization, ESI, APCI ICP, MALDI and SIMS. detectors; electron multipliers, faraday cup and microchannel plates, resolution and sensitivity. applications to ultratrace analysis, isotope ratio measurements and surface characterization.

**Unit 3** **18 Hrs**

**Potentiometry** – General principles, calomel electrodes, Ag/AgCl electrodes, membrane electrodes – ion selective electrodes, glass electrodes, liquid membrane electrodes, Clark's electrode, biosensors.

**Amperometry/Coulometry:** Basic principles, constant current and constant potential coulometry. coulometric titrations. conductometric titrations.

**Voltammetry:** Principles, voltammograms, equation of voltammogram, different waveforms—linear scan, square scan and triangular scan, cyclic voltammetry.

**Thermogravimetry:** TGA, DTA, DSC - Instrumentation, methodology, applications.

**Unit 4** **18 Hrs**

**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. UPLC, SFC LC, hyphenated techniques, LC-MS and LC MS/MS.

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

1. Various analytical methods and their applications
2. Various instrumental methods and their applications.

3. Further the student should be able to figure out the analytical process and instrumental method to be advised for a particular problem in hand

#### **SUGGESTED READINGS**

1. Skoog, D.A., Holler, F.J., and Crouch, S.R. Principles of Instrumental Analysis, 6<sup>th</sup> Edition, 2007, Thomson Learning.
2. Willard, H.H., Merritt Jr. L., Dean, J.A. and Settle, F.A. Instrumental Methods of Analysis, 7<sup>th</sup> edition, 2007, CBS Publishers.
3. Bassett, J., Denney, R.C., Jeffery, G.H., and Mendham, J. Vogel's Textbook of Quantitative Chemical Analysis, 6<sup>th</sup> Edition, 2009, Pearson Education.
4. Skoog, D.A., West, D.M., Holler, F.J., and Crouch, S.R. Fundamentals of Analytical Chemistry, 9<sup>th</sup> edition, 2013, Brooks/Cole.
5. Christian, G.D. Analytical Chemistry, 6<sup>th</sup> edition, 2004, John Wiley and Sons Inc.
6. Bard A.J. and Faulkner, I.R. Electrochemical Methods, 2<sup>nd</sup> edition, Wiley, New York, 2000.
7. Rouessac, F. and Rouessac, A. Chemical Analysis: Modern Instrumentation Methods and Techniques, 2013, John Wiley & Sons.
8. Danzer, K. Analytical Chemistry: Theoretical and Metrological Fundamentals. 2007, Springer Science & Business Media.

**Course Title: Inorganic Chemistry - I**

**Paper Code: CHL.504**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Course Objective:** To introduce theories, reaction mechanism and stability of the coordination complexes, and their magnetic and electronic properties.

**Unit 1** **12 Hrs**

**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 2** **20 Hrs**

**Reaction Mechanisms of Transition Metal Complexes**

Introduction, potential energy diagram and reactivity of metal complexes, ligand substitution reactions, substitution reactions mechanisms, 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. Marcus theory, doubly bridged inner-sphere transfer, other electron transfer reactions; two electron transfers, non-complementary reaction, ligand exchange via electron exchange, reductions by hydrated electrons, Berry pseudorotation.

**Unit 3** **20 Hrs**

Isomerism; 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, temperature independent paramagnetism (TIP) in terms of crystal field theory CFT and molecular orbital theory (MOT), quenching of orbital angular momentum by crystal fields in complexes in terms of termsplitting. effect of spin-orbit coupling and A, E & T states mixing, first order and second order Zeeman effects, spin paired and spin-free equilibria in complexes magnetic properties of polynuclear complexes involving OH, NH<sub>2</sub> and CN bridges.

**Unit 4** **20 Hrs**

**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<sup>n</sup>, d<sup>n</sup> ions, determination of the ground state terms for pn, dn, fn ions using L.S. scheme, determination of total degeneracy of terms, order of interelectronic repulsions and crystal field strength in various fields, two type of electron repulsion parameters, 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 (with help of the character table). splitting patterns of and G, H and I terms. Strong field configurations, transition from weak to strong crystal fields, evaluation of strong crystal field terms of d<sup>2</sup> configuration in octahedral and tetrahedral crystal fields (using group theory), construction of the correlation energy level diagrams of d<sup>2</sup> configuration in octahedral field, study of energy level diagrams for higher configurations, selection rules of electronic transitions in transition metal complexes, their proof using group theory, relaxation of the selection rule in centrosymmetric and non-centrosymmetric molecules, Orgel diagrams, Tanabe Sugano diagrams, calculation of 10Dq and B with use of Orgel and

Tanabe Sugano diagrams, quenching of orbitals angular momentum by ligand field, variation of the Racah parameter, central field covalency, symmetry restricted covalency, differential radial expansion, spectrochemical series, band intensities, factors influencing band widths.

**Course Outcome:** The completion of this course will enable the students to acquire knowledge of

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

#### **SUGGESTED READINGS**

1. Cotton, F.A. and Wilkinson G. Advanced Inorganic Chemistry, 6th edition, 2007, John Wiley & Sons.
2. Huheey, J. E. Inorganic Chemistry: Principles of Structure and Reactivity, 4<sup>th</sup> edition, 2006, Dorling Kindersley (India) Pvt. Ltd.
3. Greenwood, N. N. and Earnshaw, A. Chemistry of the Elements, 2<sup>nd</sup> edition, 2005 (reprinted), Butterworth-Heinemann, A division of Reed Educational & Professional Publishing Ltd.
4. Lever, A.B.P. Inorganic Electronic Spectroscopy, 2<sup>nd</sup> edition, 1984, Elsevier Science Publishers B.V.
5. Carlin, R. L. and Van Duyneveldt, A.J. Magnetic Properties of Transition Metal Compounds, Inorganic Chemistry Concepts 2, Springer-Verlag New York Inc., 1977.
6. Miessler, G. L. and Tarr, D. A. Inorganic Chemistry, 4<sup>th</sup> edition, 2011, Pearson Education.
7. Figgis, B.N. Introduction to Ligand Field, 1966 Wiley Eastern.
8. Drago, R.S. Physical Methods in Chemistry, 1965, W.B. Saunders Company.
9. Shriver, D.F.; Atkins, P.W. Inorganic Chemistry, 5<sup>th</sup> edition, 2010, Oxford University Press.
10. Earnshaw, A. Introduction to Magnetochemistry, 1968, Academic Press.
11. Dutta, R.L.; Syanal, A. Elements of Magnetochemistry, 2<sup>nd</sup> edition, 1993, Affiliated East West Press.
12. Drago, R. S. Physical Methods for Chemists, 2<sup>nd</sup> edition, 1992, Saunders College Publishing.

**Course Title: Organic Chemistry-I**

**Paper Code: CHL.506**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Course Objective:** To impart advanced knowledge of stereochemistry of organic compounds and mechanism of substitution, elimination and addition reactions.

**Unit 1** **22 Hrs**

**Stereochemistry:** IUPAC nomenclature of organic molecules, elements of symmetry, chirality, projection formulae [Flywedge, Fischer, Newman and Saw horse], configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity, racemic mixture and their resolution, configurational notations of simple molecules, D/L, R/S, E/Z and *cis/trans* configurational notations, *threo* and *erythro* isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, asymmetric synthesis, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, stereochemistry of the compounds containing nitrogen, sulphur and phosphorus, conformational analysis of 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 the course of rate of reactions, effect of conformation on reactivity, conformation of sugars, strain due to unavoidable crowding.

**Unit 2** **18 Hrs**

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

**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, Diazonium coupling.

**Unit 3** **16 Hrs**

**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 4** **16 Hrs**

**Addition to carbon-hetero multiple bonds:** Reactivity of carbonyl group, homologation and dehomologation of carbonyl compounds, Arndt-Eistert synthesis, nucleophilic addition of hetero-atoms (N,O,S), conjugate addition reactions, acylation of carbonyl carbon, carboxylic acids and derivatives, decarboxylation reactions, addition of Grignard reagent, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, mechanism of condensation reactions involving enolates-

Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions, hydrolysis of esters and amides, ammonolysis of esters.

**Course Outcome:** Students will acquire the knowledge of

1. Conformational analysis of cyclic and acyclic compounds, chirality and reactivity.
2. Mechanistic aspects in nucleophilic and electrophilic substitution.
3. Mechanistic aspects in addition and elimination reactions.

### SUGGESTED READINGS

1. Clayden, J., Greeves, N., Warren, S. and Wothers, P. Organic Chemistry, 2<sup>nd</sup> edition, 2012, Oxford University Press.
2. Finar, I.L. Organic Chemistry Volume 1, 6<sup>th</sup> edition, 2012, Pearson Education UK.
3. McMurry J. Organic Chemistry, 8<sup>th</sup> edition, 2011 Asian Book Pvt. Ltd, New Delhi
4. Smith, M. B. March's advanced organic chemistry: reactions, mechanisms, and structure, 7<sup>th</sup> Edition, 2013, John Wiley & Sons.
5. Ahluwalia, V. K. and Parashar R. K. Organic Reaction Mechanism, 4<sup>th</sup> edition, 2011, Narosa Publishing House (P) Ltd., New Delhi.
6. Bansal, R. K. A text book of Organic Chemistry, 5<sup>th</sup> edition, 2010, New Age International (P) Ltd., New Delhi.
7. Bansal R.K. Organic Reaction Mechanism, 2010, New Age International (P) Ltd., New Delhi.
8. Kalsi, P.S. Organic Reactions and Their Mechanisms. 3<sup>rd</sup> edition, 2010, New Age International, New Delhi.
9. Kalsi, P.S. Stereochemistry: Conformation and Mechanism, 2010, New Age International Ltd, New Delhi.
10. Lowry, T. H. and Richardson K. S. Mechanism and Theory in Organic Chemistry, 3<sup>rd</sup> edition, 1998, Addison-Wesley Longman Inc., New York.
11. Morrison, R.T. and Boyd, R.N. Organic Chemistry, 6<sup>th</sup> edition, 2011, Prentice- Hall of India, New Delhi.
12. Mukherjee, S.M. and Singh, S.P. Reaction Mechanism in Organic Chemistry. 3<sup>rd</sup> edition, 2009, Macmillan India Ltd., New Delhi.
13. Robert, J. D. and Casereo, M.C. Basic principle of Organic Chemistry, 2<sup>nd</sup> edition, 1977, Addison-Wesley.
14. Solomon, T.W.G, Fryhle, C.B. and Snyder, S. A. Organic Chemistry. 11<sup>th</sup> edition, 2013, John Wiley and Sons, Inc.
15. Sykes, P. A Guide Book to Mechanism in Organic Chemistry, 6<sup>th</sup> edition, 1997, Prentice Hall.
16. Eliel, E. L. and Wilen, S. H. Stereochemistry of organic compounds, 1994, John Wiley & Sons.

**Course Title: Physical Chemistry-I**

**Paper Code: CHL.508**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Course Objective:** To impart knowledge of advanced classical and statistical thermodynamics.

**Unit 1** **14 Hrs**

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

**Unit 2** **14 Hrs**

**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, real gases, fugacity, its importance and determination, standard state for gases.

**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.

**Unit 3** **16 Hrs**

**Thermodynamics of Simple Mixtures:** Thermodynamic functions for mixing of perfect gases. chemical potential of liquids. Raoult's law, Henry's law. thermodynamic functions for mixing of liquids (ideal solutions only). mixtures of volatile liquids, vapour pressure diagrams. Lever's rule, distillation diagrams. real solutions and activities, standard states for solvent and solute. stability of phases, Clapeyron equation. Clausius-clapeyron equation and its application to solid-liquid, liquid-vapour and solid-vapour equilibria.

**Unit 4** **28 Hrs**

**Statistical Thermodynamics:** The concepts of ensemble, thermodynamic probability and entropy, Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics. 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. monoatomic solids, theories of specific heat for solids.

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

1. Classical thermodynamics and understanding thermodynamic phenomenon in a chemical system
2. Statistical thermodynamics and understanding thermodynamic properties in terms of partition functions,
3. Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, theories of specific heat for solids.

**SUGGESTED READINGS**

1. Barrow, G. M. Physical Chemistry, 5<sup>th</sup> Edition, 2007, Tata McGraw-Hill.
2. Kapoor, K. L. Text Book of Physical Chemistry, Volume 2-3,5, 5<sup>th</sup>/3<sup>rd</sup> Edition, 2011, Macmillan.
3. Atkins, P. and De Paula, J. Atkins' Physical Chemistry. 9<sup>th</sup> Edition, 2009, Oxford University Press.
4. McQuarrie, D. A. and Simon, J. D. Physical Chemistry: A Molecular Approach, 1<sup>st</sup> edition, 1998, Viva Books.
5. Moore, J. W. and Pearson, R. G. Kinetics and Mechanism, 3<sup>rd</sup> edition, 1981, John Wiley and Sons.
6. Silbey, R. J. Alberty, R. A. and Bawendi, M. G. Physical Chemistry, 4<sup>th</sup> Edition, 2004, Wiley-Interscience Publication.
7. Engel, T., Reid, P. and Hehre, W. Physical Chemistry, 3<sup>rd</sup> Edition, 2012, Pearson Education.

8. Puri, B.R., Sharma L.R. and Pathania, M.S. Principles of Physical Chemistry, 46<sup>th</sup> Edition, 2013, Vishal Publishing Company.
9. Rastogi, R. P. and Mishra, R. R. An Introduction to Chemical Thermodynamics 6<sup>th</sup> edition, 2013, Vikas Publishing
10. Rajaram, J. and Kuriacose, J. C. Chemical Thermodynamics, Classical, Statistical and Irreversible Thermodynamics, 2013, Pearson Education.
11. Laurendeau N. M. Statistical Thermodynamics: Fundamentals and Applications, 2005, Cambridge University Press.
12. Nash, L. K. Elements of Statistical Thermodynamics, 2<sup>nd</sup> Edition, 2012, Dover Publication Inc.
13. Hill, T. L. An Introduction to Statistical Thermodynamics, 1986, Dover Publications Inc.



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

**Paper Code: CHP.505**

**Contact Hours: 72**

**Course Objective:** To impart knowledge of various techniques for analysis of inorganic compounds.

L	T	P	Credits	Marks
0	0	4	2	100

**Experiments:**

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

**Gravimetric Estimation**

1. Determination of  $\text{Ba}^{2+}$  as its 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.

**Spectrophotometric determination:**  $\text{NO}_3^-$  in water sample,  $\text{K}_2\text{Cr}_2\text{O}_7$  in the presence of  $\text{KMnO}_4$  and  $\text{Fe(III)}$  using 8-hydroxyquinoline.

**Flame photometric determination:** Li, Na, K and Ca.

**Atomic absorption Spectrometry:** Estimation of metals in brass, soil and groundwater.

**Course outcome:** The students will acquire knowledge of

1. Volumetric and gravimetric analysis of cations and anions.
2. Standardization and titrations of various inorganic compounds.

**SUGGESTED READINGS**

1. Pass, G. and Sutcliffe H. Practical Inorganic Chemistry, 1st edition, 1979, Chapman and Hall Ltd.
2. Jolly, W.L. Synthetic Inorganic Chemistry, 2nd edition, 1961, Prentice Hall, Inc.,.
3. Nakamoto, K. Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A and B, 5<sup>th</sup> edition, 1997, John Wiley and Sons.,.
4. Mendham, J., Denney, R.C., Barnes, J.D. and Thomas, M. Vogel's Textbook of Quantitative Chemical Analysis, 6<sup>th</sup> edition, 2000, Pearson Education Ltd.
5. Svehla, G. and Sivasankar, B. Vogel's Qualitative Inorganic Analysis (revised), 7<sup>th</sup> edition, 1996, Pearson Education Ltd.
6. Skoog, D.A., Holler, F.J., and Crouch, S.R., Principles of Instrumental Analysis, 6<sup>th</sup> Edition, 2007 Thomson Learning.

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

**Paper Code: CHP.507**

**Total Contact Hours: 72**

L	T	P	Credits	Marks
0	0	4	2	100

**Course Objective:** To develop experimental skills of various separation and purification techniques and understand various concept of stereochemistry through molecular models.

## 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, 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 and fractional distillation.

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 seven)

- 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 Preparation of Grignard reagent.
- 6 Synthesis of alcohol *via* addition of Grignard reagent to an aldehyde.
- 7 To prepare phenylpropene *via* dehydration of corresponding phenylpropanol.
- 8 Preparation of bromohydrin from phenylpropene.
- 9 To prepare ethyl cinnamate *via* acid catalyzed esterification of cinnamic acid.
- 10 Conversion of phthalic anhydride to phthalimide
- 11 Conversion of acetanilide to *p*-bromoacetanide
- 12 Conversion of *p*-bromoacetanide to *p*-bromoaniline
- 13 Synthesis of Phenytoin

### C. Demonstration of Stereochemical aspects of the compounds through molecular models.

### D. ChemDraw-Sketch:

Draw the structure of simple aliphatic, aromatic, heterocyclic organic compounds with substituents. Get the correct IUPAC name and predict the UV, IR and  $^1\text{H-NMR}$  signal analysis.

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

1. Good laboratory practices including safe handling of hazardous chemicals, laboratory glassware and equipment(s).
2. Various techniques such as thin layer chromatography, column chromatography besides extraction/workup of reaction mixture, distillation, and crystallization.
3. Importance of reaction conditions for a particular reaction and their mechanism.

4. Stereochemical aspects of the compounds through molecular model and drawing of organic structure through ChemDraw.

#### **SUGGESTED READINGS**

1. Harwood, L.M. and Moody, C.J. Experimental Organic Chemistry, 1<sup>st</sup> edition, 1989, Blackwell Scientific Publishers.
2. Vogel, A.I. Textbook of Practical Organic Chemistry, 6<sup>th</sup> edition, 1978, ELBS, Longman Group Ltd.
3. Mann, F.G. and Saunders, B.C. Practical Organic Chemistry, 4<sup>th</sup> edition, New Impression, 1975, Orient Longman Pvt. Ltd.
4. Leonard, J. and Lygo, B. Advanced Practical Organic Chemistry, 1995, Chapman and Hall.
5. Armarego, W. L. and Chai, C. Purification of Laboratory Chemicals, 2012, Butterworth-Heinemann.
6. Young, J. A. Improving safety in the chemical laboratory: a practical guide. 2<sup>nd</sup> Edition, 1991, Wiley Publishing.

**Course Title: Inorganic Chemistry-II**

**Paper Code: CHL.521**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Course Objective:** To introduce the concepts and importance of symmetry and group theory in solving chemical problems and clusters of boranes, organometallics, inorganic chains, rings and cages.

**Unit 1** **12 Hrs**

**Symmetry**

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

**Unit2** **20 Hrs**

**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, qualitative splitting of s, p, d, f orbitals in octahedral, tetrahedral and square planar fields using character tables and without the use of character tables. ligands symmetry orbitals and metal orbitals involved in molecular orbitals formation in octahedral complexes, MO diagrams for octahedral tetrahedral and square planar complexes showing  $\sigma$  and  $\pi$  bonding in transition metal complexes

**Unit 3** **20 Hrs**

**Metal Complexes**

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

**Unit 4** **20 Hrs**

**Inorganic chains, rings and cages**

- a) **Chains:** Catenation, heterocatenation, isopolyanions and heteropolyanions.
- b) **Rings:** Borazines, phosphazenes, other heterocyclic inorganic ring systems, homocyclic inorganic systems.
- c) **Cages:** Cage compounds having phosphorus, oxygen, nitrogen and sulphur: boron cage compounds, boranes, carboranes and metallocenecarboranes.

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

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

**SUGGESTED READINGS**

1. Cotton, F.A.; Wilkinson Advanced Inorganic Chemistry, 6<sup>th</sup> edition, 2007, John Wiley & Sons.

2. Huheey, J. E. Inorganic Chemistry: Principles of Structure and Reactivity, 4<sup>th</sup> edition, 2006, Dorling Kindersley (India) Pvt. Ltd.
3. Greenwood, N.N. and Earnshaw, A. Chemistry of the Elements, 2<sup>nd</sup> edition, 2005 (reprinted), Butterworth-Heinemann, A division of Read Educational & Professional Publishing Ltd.
4. Lever, A.B.P. Inorganic Electronic Spectroscopy, 2<sup>nd</sup> edition, 1984, Elsevier Science Publishers B.V.
5. Carlin, R. L. and Van Duyneveldt, A.J. Magnetic Properties of Transition Metal Compounds, Inorganic Chemistry Concepts 2, Springer-Verlag New York Inc., 1977.
6. Shriver, D.F.; Atkins, P.W. Inorganic Chemistry, 5<sup>th</sup> edition, 2010, Oxford University Press.
7. Earnshaw, A. Introduction to Magnetochemistry, 1968, Academic Press.
8. Dutta, R.L.; Syanal, A. Elements of Magnetochemistry, 2<sup>nd</sup> edition, 1993, Affiliated East West Press.
9. Drago, Russell S. *Physical Methods for Chemists*, 2<sup>nd</sup> edition, 1992, Saunders College Publishing

**Course Title: Organic Chemistry-II**

**Paper Code: CHL.523**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Course Objective:** To impart knowledge of pericyclic and photochemical reactions, Molecular rearrangements and aromaticity.

**Unit 1** **16 Hrs**

**Reactive intermediates:** Generation, structure and reactions of carbocation, carbanion, 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, Huckel's rule, energy level of  $\pi$ -molecular orbitals, annulenes, azulenes, antiaromaticity.

**Unit 2** **16 Hrs**

**Photochemistry:** Franck-Condon principle, Jablonski diagram, singlet and triplet states, photosensitization, quantum efficiency, photochemistry of carbonyl compounds, Norrish type-I and type-II cleavages, 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 3** **22 Hrs**

**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 and (iii) Huckel-Mobius aromatic and antiaromatic transition state method.

**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 and (iii) Huckel-Mobius aromatic and antiaromatic transition state method.

**Sigmatropic reactions:** [1,j] and [i,j] shifts; suprafacial and antarafacial, selection rules for [l] shifts; Cope and Claisen rearrangements; explanation for the mechanism by (i) symmetry properties of HOMO (ii) Huckel-Mobius aromatic and antiaromatic transition state method; introduction to cheletropic reactions and the explanation of mechanism by FMO theory.

**Unit 4** **18 Hrs**

**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, Schmidt, Baeyer-Villiger, Shapiro reaction, Carroll, Claisen, Cope, Gabriel-Colman, Smiles and Sommelet-Hauser rearrangements.

**Selective Name Reactions:** Sharpless asymmetric epoxidation, dihydroxylation, Ene/Alder-ene reaction, Dakin reaction, Reformatsky, Robinson annulation, Michael addition, Stork-enamine, Hofmann-Löffler Fretag, Shapiro reaction, Chichibabin reaction.

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

1. Basic principles of photochemical reactions, photochemistry of carbonyl and aromatic compounds.
2. Various thermally or photochemically driven pericyclic reactions and explanation for their stereochemical aspects.
3. Various molecular rearrangement and their application in organic synthesis for the conversion of different functional group.
4. Aromaticity and antiaromaticity in carbocyclic and heterocyclic compounds.

### SUGGESTED READINGS

1. Acheson, R.M. An introduction to the Chemistry of Heterocyclic Compounds, 3<sup>rd</sup> edition, 1976 Wiley India Pvt. Ltd.
2. Clayden, J., Greeves, N., Warren, S. and Wothers, P. Organic Chemistry, 2<sup>nd</sup> edition, 2012, Oxford University Press.
3. Ahluwalia, V. K. and Parasar R. K. Organic Reaction Mechanism, 4<sup>th</sup> edition, 2011, Narosa Publishing House (P) Ltd., New Delhi.
4. Bansal, R. K. A text book of Organic Chemistry, 5<sup>th</sup> edition, 2010, New Age International (P) Ltd., New Delhi.
5. Bansal R.K. Organic Reaction Mechanism, 2010, New Age International (P) Ltd., New Delhi.
6. Bansal, R.K. Heterocyclic Chemistry, 5<sup>th</sup> edition, 2010, New Age International (P) Ltd., New Delhi.
7. Carey B. F. A., Sundberg R.J., Advanced Organic Chemistry Part A, 4<sup>th</sup> edition, 2002, Kluwer Academic Publishers.
8. Carey B. F. A., Sundberg R.J., Advanced Organic Chemistry Part B, 5<sup>th</sup> edition, 2007, Springer Science and Business Media Ltd.
9. Finar, I.L. Organic Chemistry Volume 1, 6<sup>th</sup> edition, 2012, Pearson Education UK.
10. Gilchrist, T.L. (1997). Heterocyclic Chemistry, 3<sup>rd</sup> edition, 1997, Addison Wesley Longman Publishers, US.
11. Gupta R.R., Kumar M. and Gupta V. Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3, 2010, Springer Verlag, India.
12. Joule, J.A. and Mills, K. Heterocyclic Chemistry, 5<sup>th</sup> edition, 2010, Blackwell Publishers, New York.
13. Kalsi, P.S. Organic Reactions and Their Mechanisms. 3<sup>rd</sup> edition, 2010, New Age International, New Delhi.
14. Lowry, T. H. and Richardson K. S. Mechanism and Theory in Organic Chemistry, 3<sup>rd</sup> edition, 1998, Addison-Wesley Longman Inc., New York.
15. Morrison, R.T. and Boyd, R.N. Organic Chemistry, 6<sup>th</sup> edition, 2011, Prentice- Hall of India, New Delhi.
16. Mukherjee, S.M. and Singh, S.P. Reaction Mechanism in Organic Chemistry. 3<sup>rd</sup> edition, 2009, Macmillan India Ltd., New Delhi.
17. Katritzky, A. R., Ramsden, C. A., Joule, J. A. and Zhdankin V. V. Handbook of Heterocyclic Chemistry, 3<sup>rd</sup> edition, 2010, Elsevier UK.
18. Smith, M. B. March's advanced organic chemistry: reactions, mechanisms, and structure, 7<sup>th</sup> Edition, 2013, John Wiley & Sons.
19. Sykes, P. A Guide Book to Mechanism in Organic Chemistry, 6<sup>th</sup> edition, 1997, Prentice Hall.
20. Norman, R.O.C. and Coxon, J.M. Principles of Organic Synthesis, 3<sup>rd</sup> edition, 1998, Nelson Thornes, Blackie Academic & Professional.

**Course Title: Physical Chemistry-II****Paper Code: CHL.524****Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Course objective:** To impart knowledge of applications of electrochemistry, reaction kinetics, surface reaction, adsorption and catalysis.

**Unit 1** **18 Hrs**

**Electrochemistry:** Nernst equation, electrochemical series, electrochemical cells, concentration cells with and without liquid junction, application of electrochemical cell, thermodynamics of reversible electrodes and reversible cells. zeta potential, redox indicators, activity-coefficients, mean activity coefficients; Debye-Huckel treatment of dilute electrolyte solutions, derivation of Debye-Huckel limiting law, extended Debye-Huckel law, photoelectrochemical cells, conductometric and potentiometric titrations.

**Unit 2** **18 Hrs**

**Reaction Kinetics:** Introduction, rates of chemical reactions, methods of determining rate laws, mechanisms of chemical reactions and steady state approximation, laws of photochemistry, kinetics of photochemical and composite reactions, chain and oscillatory reactions, collision and transition state theories, steric factor, treatment of unimolecular reactions, ionic reactions: salt effect.

**Unit 3** **18 Hrs**

**Fast Reaction:** Introduction to fluorescence, phosphorescence and luminescence, Jablonski diagram, Steady state and time resolved emission, quantum yield, 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, measurement of fluorescence and phosphorescence lifetimes, photoinduced electron transfer rates.

**Unit 4** **18 Hrs**

**Adsorption:** Adsorption of solids, Gibbs adsorption isotherm, BET adsorption isotherm: estimation of surface area of solids, Langmuir and Freundlich Isotherms.

**Catalysis:** Homogeneous catalysis and heterogeneous catalysis, enzyme catalysis. Effect of pressure on reaction rate, Kinetics of catalytic reactions, Kinetics of surface reaction.

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

1. Redox processes in electrochemical systems, Debye-Huckel theory and determination of activity and activity coefficient.
2. Mechanism for chemical reactions for optimizing the experimental conditions,
3. Kinetics of fast reactions by ultrafast methods and techniques
4. Application of homogeneous and heterogeneous catalysis in chemical synthesis
5. Importance of adsorption process and catalytic activity at the solid surfaces

**SUGGESTED READINGS**

1. Barrow, G. M. Physical Chemistry, 5<sup>th</sup> Edition, 2007, Tata McGraw-Hill.
2. Kapoor, K. L. Text Book of Physical Chemistry, Volume 1, 4, 5<sup>th</sup> Edition, 2011, MACMILLAN,.
3. Atkins, P. and De Paula, J. Atkins' Physical Chemistry. 9<sup>th</sup> Edition, 2009, Oxford University Press.
4. McQuarrie, D. A. and Simon, J. D. Physical Chemistry: A Molecular Approach, 1<sup>st</sup> edition, 1998, Viva Books,.



5. Moore, J. W. and Pearson, R. G. Kinetics and Mechanism, 3<sup>rd</sup> edition, 1981, John Wiley and Sons.
6. Silbey, R. J. Alberty, R. A. and Bawendi, M. G. Physical Chemistry, 4<sup>th</sup> Edition, 2004, Wiley-Interscience Publication.
7. Engel T., Reid, P. and Hehre, W. Physical Chemistry, 3<sup>rd</sup> Edition, 2012, Pearson Education.
8. Puri, B.R. Sharma L.R. and Pathania M.S. Principles of Physical Chemistry, 46<sup>th</sup> Edition, 2013, Vishal Publishing Company.
9. Laidler, K. J. Chemical Kinetics, 3<sup>rd</sup> Edition, 1987, Pearson Education Ltd.
10. Engel T. and Reid, P. Thermodynamics, Statistical Thermodynamics, & Kinetics, 3<sup>rd</sup> edition, 2013, Pearson Education.
11. Lakowicz, J. R. Principles of Fluorescence Spectroscopy, 3<sup>rd</sup> edition, 2006, Springer.
12. Raj, G. Surface Chemistry (Adsorption), 4<sup>th</sup> Edition, 2002, Goel Publishing House.

L	T	P	Credits	Marks
4	1	0	4	100

**Course Title: Quantum Chemistry**

**Paper Code: CHL.526**

**Total Lectures: 72**

**Course objective:** To acquire knowledge of the quantum chemical description of chemical bonding, reactivity and their applications in molecular spectroscopy and inorganic chemistry.

### Unit 1 18 Hrs

**Fundamental Background:** Postulates of quantum mechanics, eigen values and eigen functions, operators, hermitian and Unitary operators, some important theorems. Schrodinger equation-particle in a box (1D, 3D) and its application, potential energy barrier and tunnelling effect, one-dimensional harmonic oscillator and rigid rotor, particle in a ring, hydrogen atom.

### Unit 2 18 Hrs

**Approximate Methods:** Perturbation theory for non-degenerate and degenerate states and its applications. The variation theorem and its application.

### Unit 3 18 Hrs

**Angular Momentum:** Ordinary angular momentum, eigen functions and eigen values for angular momentum, addition of angular momenta, spin, antisymmetry and Pauli exclusion principle.

**Electronic Structure of Atoms:** electronic configuration, Russell-Saunders terms and coupling schemes, magnetic effects: spin-orbit coupling and Zeeman Splitting, the self-consistent field method, Hartree-Fock SCF method for molecules.

### Unit 4 18 Hrs

**Born-Oppenheimer Approximation:** LCAO-MO and VB treatments of the  $H_2^+$  and  $H_2$ , hybridization and valence MOs of  $H_2O$  and  $NH_3$ . Huckel Theory of acyclic and cyclic conjugated systems, bond order and charge density calculations.

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

1. Schrodinger equation for a particle in a box and quantum chemical description.
2. Electronic and Hamiltonian operators for molecules.
3. Quantum chemical description of angular momentum and term symbols for a one and many-electron systems.
4. Born-Oppenheimer approximation, the Pauli principle, Hund's rules, Hückel theory and the variation principle.

### SUGGESTED READINGS

1. Levine, I.N. Quantum Chemistry, 5<sup>th</sup> edition, 2000, Pearson Educ., Inc. New Delhi.
2. Chandra, A.K. Introductory Quantum Chemistry, 4<sup>th</sup> Edition, 1994, Tata Mcgraw Hill.
3. Prasad, R.K., Quantum Chemistry, 4<sup>th</sup> Edition, 2009, New Age Science.
4. McQuarrie, D. A. and Simon, J. D. Physical Chemistry: A Molecular Approach, 1<sup>st</sup> edition, 1998, Viva Books.
5. Murrell, J.N., Kettle S.F.A. and Tedder, J. M. Valence Theory, 2<sup>nd</sup> edition, 1965, John Wiley.
6. Lowe, J. P. and Peterson, K. Quantum Chemistry, 3<sup>rd</sup> Edition, 2006, Academic Press.

**Course Title: Practical Inorganic Chemistry -II****Paper Code: CHL.522****Total Lectures: 72**

L	T	P	Credits	Marks
0	0	4	2	100

**Course objective:** To teach the synthesis of inorganic complexes and their characterization with instrumental techniques.

1. Preparation of Chloropentaammine cobalt (III) Chloride and its IR measurements.
2. Preparation of  $[\text{Co}(\text{en})_2\text{Cl}_2] \text{Cl}$ ,  $\text{Na}_2 [\text{Fe}(\text{CN})_5 \text{NH}_3] \cdot \text{H}_2\text{O}$ ,  $[\text{UO}_2(\text{NO}_3)_2 \text{Py}_2] \cdot \text{Cu}_2(\text{CH}_3\text{COO})_4(\text{H}_2\text{O})_2$ .
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-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 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

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

1. Preparation and purification of different inorganic complexes.
2. Application of UV-Vis, FT-IR, Magnetic moment measurement, Conductivity measurements, NMR and Thermogravimetric analysis for characterization of coordination complexes.

**SUGGESTED READINGS**

1. Pass, G. and Sutcliffe H. Practical Inorganic Chemistry, 1<sup>st</sup> edition, 1979, Chapman and Hall Ltd.
2. Jolly, W.L. Synthetic Inorganic Chemistry, 2<sup>nd</sup> edition, 1961, Prentice Hall, Inc.,.
3. Nakamoto, K. Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A and B, 5<sup>th</sup> edition, 1997, John Wiley and Sons,.
4. Mendham, J., Denney, R.C., Barnes, J.D. and Thomas, M. Vogel's Textbook of Quantitative Chemical Analysis, 6<sup>th</sup> edition, 2000, Pearson Education Ltd.
5. Kolthoff, I.M. and Sandell, E.B. Text Book of Quantitative Inorganic Analysis, Revised Edition, 1968, London Macmillan and Co. Ltd.
6. Marr, G. and Rockett, B.W. Practical Inorganic Chemistry, 1972, John Wiley & Sons.
7. Jolly, W.L. The Synthesis and Characterization of Inorganic Compounds. 1970, Prentice Hall Press.

**Course Title: Practical Physical Chemistry-II****Paper Code: CHL.525****Total Contact Hours: 72**

L	T	P	Credits	Marks
0	0	4	2	100

**Course objective:** To impart knowledge and hand-on experiences of different analytical techniques for chemical analysis

1. Determination of strength of a given base by titrating with an acid conductometrically.
2. Determination of solubility and solubility product of sparingly soluble salts (e.g.,  $\text{PbSO}_4$ ,  $\text{BaSO}_4$ ) conductometrically.
3. Determination standard electrode potential of  $\text{Fe}^{2+}/\text{Fe}^{3+}$  system by potentiometer using potassium permanganate solution.
4. Determination of pKa of acetic acid and glycine by pH meter using NaOH.
5. Determination of relative and absolute viscosity of a given liquid.
6. Determination of surface tension of alcohols.
7. Determination of refractive indices of given liquids.
8. Determination of concentrations of heme proteins using spectrophotometer
9. Preparation of buffers and measurement of their pH
10. Verification of the Lambert Beer's law.
11. Structural analysis of amino acids and proteins using FTIR and CD spectrometer.
12. Determination of the  $T_m$  values of DNA and proteins.
13. Study of the thermal/cold denaturations of proteins using UV-visible and CD spectroscopic techniques.
14. Molecular weight of a non-electrolyte by cryoscopy method.
15. Determination of stability constant of Fe(III)-salicylic acid complex by spectrophotometer.

**Course Outcome:** The students will acquire knowledge of development of experimental skills on conductivity meter, potentiometer, pH meter, viscometer, refractometer, spectrophotometer, CD and FTIR for different applications.

**SUGGESTED READINGS**

1. Nad, A. K., Mahapatra, B. and Ghoshal, A. An Advanced Course in Practical Chemistry, 2014, New Central Book Agency (P) Ltd.
2. Maity S. and Ghosh, N. Physical Chemistry Practical, 2012, New Central Book Agency (P) Ltd.
3. Elias, A. J. Collection of Interesting General Chemistry Experiments, 2008, Universities Press.
4. Khosla, B.D., Garg, V.C., and Gulati A.R., Senior Practical Physical Chemistry, 2007, S. Chand & Sons.
5. Yadav, J.B. Advanced Practical Physical Chemistry, 2008, Krishna Prakasan Media.
6. Das, R.C. and Behra, B. Experimental Physical Chemistry, 1983, Tata McGraw-Hill.
7. James, A.M. and Prichard, F.E. Practical Physical Chemistry, 3<sup>rd</sup> edition, 1974, Longman, Harlow.
8. Ghosh, J.C., Experiments in Physical Chemistry, 1990, Bharati Bhavan.

**Course Title: Seminar**

**Paper Code: CHS.599**

**Total Contact Hours: 36**

L	T	P	Credits	Marks
0	2	0	2	100

**Course objective:** The course would develop scientific aptitude, critical thinking, research writing and research presentation.

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.

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

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

**Course Title: Inorganic Chemistry-III****Paper Code: CHL.601****Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Course objective:** To aware the knowledge of coordination chemistry and properties of f-block elements, role of metals in bioinorganic chemistry, and spectroscopic techniques to analyse the inorganic compounds

**Unit 1** **28 Hrs****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, organo lanthanides and actinides, separation of lanthanides and actinides, analytical application of lanthanides and actinides-lanthanides as shift reagents and high temperature super conductors, manmade elements-theoretical background, production, separation and predicted properties.

**Unit 2** **20 Hrs**

**Bioinorganic Chemistry:** Heme and non-heme proteins, haemoglobin and myoglobin as oxygen carriers, bohr effect, relaxed and tense (R & T) configurations of haemoglobin, structure and functions of cytochromes, hemerythrins and hemocyanins. biochemistry of iron, iron storage and transport, and ferritin, transferrin., blue copper proteins, zinc protein (carbonic anhydrase), and iron-sulfur proteins, metal deficiency and disease, toxic effects of metals.

**Unit 3** **12 Hrs****Nuclear Magnetic Resonance (NMR) and Electron Spin Resonance (ESR) Spectroscopy:**

**NMR:** The contact and pseudo contact shifts , factors affecting nuclear relaxation , some applications including biochemical systems , an overview of NMR of metal nuclides with emphasis on  $^{195}\text{Pt}$  and  $^{119}\text{Sn}$  NMR. **ESR:** Hyperfine coupling, 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 and to inorganic free radicals such as  $\text{PH}_4$  ,  $\text{F}_2$  and  $[\text{BH}_3]$ -

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

**Unit 4** **12 Hrs****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.

**Vibrational Spectroscopy**

Symmetry and shapes of  $\text{AB}_2$ ,  $\text{AB}_3$ ,  $\text{AB}_4$ ,  $\text{AB}_5$  and  $\text{AB}_6$  mode of bonding of ambidentate ligands, ethylenediamine and diketonato complexes, applications of resonance Raman spectroscopy particularly for the study of active sites of metalloproteins.

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

1. Details on f-block elements properties
2. Structure and biological functions of proteins and the role of metals in biology
3. Structural support to inorganic compounds through spectroscopic techniques

## SUGGESTED READINGS

1. Drago, Russell S. Physical Methods for Chemists, 2<sup>nd</sup> edition, 1992, Saunders College Publishing.
2. Ebsworth, E.A.V., Rankin, D.W.H. and Cracock, S. Structural Methods in Inorganic Chemistry, 1st edition, 1987, ELBS.
3. Cotton, F.A. and Lippard, S.J. Progress in Inorganic Chemistry, Vol. 8, Vol. 15, Wiley Internationals.
4. Lever, A.B.P. Inorganic Electronic Spectroscopy, 2<sup>nd</sup> edition, 1984, Elsevier Science Publishers B.V.
5. Parish, R.V. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, 1st edition, 1990, Ellis Harwood.
6. Silverstein, R.M. Bassler, G.C. and Morrill, T.C. Spectrometric Identification of Organic Compounds, 6<sup>th</sup> edition, 2002, John Wiley.
7. Abraham, R.J., Fisher, J. and Loftus, P. Introduction to NMR Spectroscopy, Wiley.
8. Dyer, J.R. Application of Spectroscopy of Organic Compounds, Prentice Hall.
9. Nakamoto, K. Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A and B, 5<sup>th</sup> edition, 1997, John Wiley and Sons.
10. Carlin, R.I. Transition Metal Chemistry, Vol. 3, Marcell Dekker Publication
11. Martin, M.L., Delpuech, J.J. and Martin, G.J. Practical NMR Spectroscopy, Heyden.
12. Williams, D.H. and Fleming, I. Spectroscopic Methods in Organic Chemistry, Tata McGraw-Hill.
13. Greenwood, N. N. and Earnshaw, A. Chemistry of the Elements, 1984.
14. Ozin, G. A., Arsenault, A. C. and Cademartiri L. Nanochemistry: a chemical approach to nanomaterials, 2009, Royal Society of Chemistry.
15. Klabunde, Kenneth J., and Ryan M. Richards, eds. Nanoscale materials in chemistry 2009, John Wiley & Sons.

**Course Title: Organic Chemistry-III**

**Paper Code: CHL.602**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Course objective:** To impart knowledge of certain topics in Chemistry such as structure and reactivity, retrosynthetic analysis, reagents for oxidation and reduction and heterocyclic chemistry.

**Unit 1** **16 Hrs**

**Reaction mechanism, structure and reactivity:** Types of mechanisms, types of reactions, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotopes effects, effect of structure on reactivity; resonance, inductive, electrostatic and steric effect, quantitative treatment, the hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation.

**Unit 2** **18Hrs**

**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 in 1,2-, 1,3-, 1,4 & 1,5-difunctional compounds, use of acetylenes and aliphatic nitro compounds in organic synthesis, two group c-c disconnections, diels-alder reaction, 1,3-difunctionalised compounds, control in carbonyl condensation, 1,5-difunctionalised compounds.

**Unit 3** **18 Hrs**

**Metal and non-metal mediated oxidation and reductions:** Mechanism, selectivity, stereochemistry and applications of oxidation reactions, Oppenauer oxidation, oxidation reactions using DDQ, NBS, Pb(OAc)<sub>4</sub>, Selenium dioxide, DCC, PCC, PDC, CAN, Cr and Mn reagents, Periodic acid, OsO<sub>4</sub>, Swern oxidations, hydroboration, ozonolysis, epoxidations using peracids, Des-Martin periodinate.

Mechanism, selectivity, stereochemistry and applications of catalytic hydrogenations using Pd, Pt and Ni catalysts, Clemmensen reduction, Wolff-Kishner reduction, Meerwein-Ponndorf-Verley reduction, dissolving metal reductions, metal hydride reductions using NaBH<sub>4</sub>, LiAlH<sub>4</sub>, DIBAL. Wilkinson's catalysis, boron in reduction, Birch reduction.

**Unit 4** **20 Hrs**

**Heterocyclic Chemistry:** Systematic nomenclature (Hantzsch-Widman system) 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 and their synthesis

**Three-membered and four-membered heterocycles:** synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes and thietanes.

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

**Benzo-fused five-membered and six membered heterocycles:** indoles, benzofurans and benzimidazoles, benzothiazoles, imidazopyridine, pyrrolopyridine/pyrimidines.

**Six-membered heterocycles:** Synthesis and reactions of pyrylium salts and pyrones, coumarins, chromones, pyridine, pyrimidine *etc.*

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



1. Various reaction mechanisms including effect of structure on reactivity besides kinetic and thermodynamic controlled reactions.
2. Designing a retrosynthetic approach for the synthesis of a target molecule.
3. Oxidation and reduction reagents and their application for functional group conversion in organic synthesis.
4. Nomenclature, synthesis and reactivity of smaller, five and six membered heterocyclic compounds.

### SUGGESTED READINGS

1. Acheson, R.M. An Introduction to the Chemistry of Heterocyclic Compounds, 3<sup>rd</sup> edition, 1976 Wiley India Pvt. Ltd.
2. Ahluwalia, V. K. and Parasar R. K. Organic Reaction Mechanism, 4<sup>th</sup> edition, 2011, Narosa Publishing House (P) Ltd., New Delhi.
3. Bansal, R. K. A text book of Organic Chemistry, 5<sup>th</sup> edition, 2010, New Age International (P) Ltd., New Delhi.
4. Bansal R.K. Organic Reaction Mechanism, 2010, New Age International (P) Ltd., New Delhi.
5. Bansal, R.K. Heterocyclic Chemistry, 5<sup>th</sup> edition, 2010, New Age International (P) Ltd., New Delhi.
6. Carey B. F. A., Sundberg R.J., Advanced Organic Chemistry Part A, 4<sup>th</sup> edition, 2002, Kluwer Academic Publishers.
7. Carey B. F. A., Sundberg R.J., Advanced Organic Chemistry Part B, 5<sup>th</sup> edition, 2007, Springer Science and Business Media Ltd.
8. Finar, I.L. Organic Chemistry Volume 1, 6<sup>th</sup> edition, 2012, Pearson Education UK.
9. Gilchrist, T.L. Heterocyclic Chemistry, 3<sup>rd</sup> edition, 1997, Addison Wesley Longman Publishers, US.
10. Gupta R.R., Kumar M. and Gupta V. Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3, 2010, Springer Verlag, India.
11. Joule, J.A. and Mills, K. Heterocyclic Chemistry, 5<sup>th</sup> edition, 2010, Blackwell Publishers, New York.
12. Kalsi, P.S. Organic Reactions and Their Mechanisms. 3<sup>rd</sup> edition, 2010, New Age International, New Delhi.
13. Kalsi, P. S. Stereochemistry: Conformation and Mechanism, 7<sup>th</sup> edition, 2008, New Age International (P) Ltd., India.
14. Lowry, T. H. and Richardson K. S. Mechanism and Theory in Organic Chemistry, 3<sup>rd</sup> edition, 1998, Addison-Wesley Longman Inc., New York.
15. Morrison, R.T. and Boyd, R.N. Organic Chemistry, 6<sup>th</sup> edition, 2011, Prentice-Hall of India, New Delhi.
16. Mukherjee, S.M. and Singh, S.P. Reaction Mechanism in Organic Chemistry. 3<sup>rd</sup> edition, 2009, Macmillan India Ltd., New Delhi.
17. Katritzky, A. R., Ramsden, C. A., Joule, J. A. and Zhdankin V. V. Handbook of Heterocyclic Chemistry, 3<sup>rd</sup> edition, 2010, Elsevier UK.
18. Smith, M. B. March's advanced organic chemistry: reactions, mechanisms, and structure, 7<sup>th</sup> Edition, 2013, John Wiley & Sons.
19. Warren, S., Organic synthesis: The Synthons Approach 2010, John Wiley & Sons, New York.
20. Warren, S. And Wyatt, P. Designing Organic synthesis: A Disconnection Approach. 2<sup>nd</sup> Edition, 2010, John Wiley & Sons, New York.
21. Corey, E.J. and Cheng X.-M. The Logic of Chemical Synthesis, 1989, John Wiley & Sons.

**Course Title: Physical Chemistry-III**

**Paper Code: CHL.604**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Course objective:** To impart the knowledge of electronic, rotation, vibration, laser, Mossbauer, NMR, FTIR, ESR spectroscopy and their applications.

**Unit 1** **18Hrs**

**Unifying Principles:** Electromagnetic radiation, interaction of electromagnetic radiation with matter, line width, selection rules, intensity of spectral lines, rotational, vibrational and electronic energy levels.

**Electronic Spectroscopy:** Energies of atomic and molecular orbitals, UV-Visible spectra, spectra of hydrogen atom and alkali metal atoms, applications, Franck-Condon principle, electronic spectra of polyatomic molecules.

**Lasers and Laser Spectroscopy:** Principles of laser action, pulsed lasers, Q-switching, harmonic generation, examples of lasers: He-Ne, Nd-YAG, dye lasers, femtosecond spectroscopy.

**Unit 2** **18 Hrs**

**Microwave Spectroscopy:** Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor, Stark effect, applications.

**Mossbauer Spectroscopy:** Basic principles, application of the technique to the studies of (1) bonding, structures and oxidation state of  $\text{Fe}^{+2}$  and  $\text{Fe}^{+3}$  compounds.

**Unit 3** **18 Hrs**

**Vibrational Spectroscopy:** Infrared Spectroscopy– Simple harmonic oscillator, Vibrational energies of diatomic molecules, Anharmonicity, Vibration-rotation spectroscopy, P, Q, R branches, Vibrations of polyatomic molecules, Group frequencies, Overtones, Hot bands, Applications.

**Raman Spectroscopy** - Classical and quantum theories of Raman Effect, pure rotational, vibrational and vibrational-rotational raman spectra, mutual exclusion principle, coherent anti stokes raman spectroscopy.

**Unit 4** **18 Hrs**

**Nuclear Magnetic Resonance (NMR) Spectroscopy:** Basic principles, instrumentation, magnetization vector and relaxation, nmr transitions, bloch equation, relaxation effects and mechanism, shielding and deshielding of magnetic nuclei, chemical shift, spin-spin interactions and coupling constant 'J', double resonance and spin tickling, effect of quadrupole nuclei, nuclear overhauser effect (NOE), multiple pulse methods, nmr in medical diagnostics.

**Electron Spin Resonance Spectroscopy** - Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value, hyperfine coupling constants, instrumentation and applications.

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

1. Microwave, Infrared-Vibration-rotation Raman and infra-red Spectroscopy and their applications for chemical analysis
2. Mossbauer Spectroscopy and their applications
3. Electronic spectroscopy of different elements and simple molecules.
4. Nuclear Magnetic and Electron Spin Resonance Spectroscopy for organic compounds analysis, medical diagnostics.

**SUGGESTED READINGS**

1. Hollas, J. M. Modern Spectroscopy, 4<sup>th</sup> edition, 2004, John Wiley & Sons, Ltd.
2. Barrow, G. M. Introduction to Molecular Spectroscopy, 1988, McGraw-Hill International.
3. Banwell C. N. and McCash, E.M. Fundamentals of Molecular Spectroscopy, 4<sup>th</sup> edition, 1994, Tata McGraw Hill, New Delhi.
4. Lakowicz, J. R. Principles of Fluorescence Spectroscopy, 3<sup>rd</sup> edition, 2006, Springer.
5. Carrington A. and Mc Lachlan, A. D. Introduction to Magnetic Resonance, 1979, Chapman and Hall, London.
6. Harris, R. K. Nuclear Magnetic Resonance Spectroscopy, 1986, Addison-Wesley Longman Ltd, London.
7. Windawi, H. and Floyd, F.L.H. Applied Electron Spectroscopy for Chemical Analysis, Chemical Analysis, Vol. 63: A Series of Monographs on Analytical Chemistry and Its Applications Series, 1982, John Wiley.
8. Parish, R.V., NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, 1991, Ellis Harwood.
9. Chang, R. Basic Principles of Spectroscopy, 1971, McGraw-Hill.
10. Ghosh, P.K. Introduction to Photoelectron Spectroscopy, Chemical Analysis Vol. 67: A Series of Monographs on Analytical Chemistry and Its Applications Series, 1983, John Wiley & Sons, New York.
11. Gunther, H. NMR Spectroscopy: Basic Principles, Concepts, and Application in Chemistry, 3<sup>rd</sup> Edition, 2013, Wiley Publishing.
12. Carrington, A. and MacLachlan, A.D. Introduction to Magnetic Resonance, 1967, Harper and Row, New York, USA.
13. Barrow, G. M. Physical Chemistry, 5<sup>th</sup> Edition, 2007, Tata McGraw-Hill.
14. Kapoor, K. L. Text Book of Physical Chemistry, Volume 1, 4, 5<sup>th</sup> Edition, 2011, MACMILLAN.
15. Atkins, P. and De Paula, J. Atkins' Physical Chemistry. 9<sup>th</sup> Edition, 2009, Oxford University Press.
16. McQuarrie, D. A. and Simon, J. D. Physical Chemistry: A Molecular Approach, 1<sup>st</sup> edition, 1998, Viva Books.
17. Silbey, R. J. Alberty, R. A. and Bawendi, M. G. Physical Chemistry, 4<sup>th</sup> Edition, 2004, Wiley-Interscience Publication.

**Course Title: Spectral Analysis**

**Paper Code: CHL.606**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Course objective:** To introduce the principles of various spectroscopic techniques such as UV, IR, NMR and Mass spectroscopy and illustrate their application for structural elucidation of organic molecules.

**Unit 1** **18 Hrs**

**UV-Visible spectroscopy:** Principle of UV-Visible spectroscopy, role of solvents, chromophores and their interaction with UV-visible radiation and their utilization in structural, qualitative and quantitative analysis of drug molecules. Woodward-Fieser rule, stereochemical aspects.

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

**Unit 2** **18Hrs**

**Nuclear magnetic resonance spectroscopy:** Magnetic properties of nuclei, field and precession, chemical shift concept, isotopic nuclei, reference standards and solvents. <sup>1</sup>H- nmr spectra, chemical shifts, spin spin coupling, coupling constants, integration of signals, interpretation of spectra, decoupling, double resonance and shift reagent methods, long range coupling, resonance of other nuclei e.g. <sup>19</sup>F, <sup>15</sup>N, <sup>31</sup>P.

**Unit 3** **18Hrs**

Principles of FT-NMR with reference to <sup>13</sup>C NMR, free induction decay, average time domain and frequency domain signals, spin-spin and spin-lattice relaxation phenomenon, nuclear overhauser enhancement (NOE), <sup>13</sup>C NMR spectra, their interpretation and application. DEPT techniques, Principle of 2-D NMR, Correlation spectroscopy (COSY) Homo COSY (<sup>1</sup>H-<sup>1</sup>H COSY), Hetro COSY (<sup>1</sup>H-<sup>13</sup>C COSY, HMQC), long range <sup>1</sup>H-<sup>13</sup>C COSY (HMBC), NOESY

**Unit 4** **18Hrs**

**Mass spectrometry:** Basic principles and brief outline of instrumentation, Ion formation, molecular ion, metastable ion, McLafferty rearrangement, nitrogen rule, fragmentation process in relation to molecular structure and functional groups. relative abundance of isotopes, chemical ionization, FAB, ESI and MALDI other recent advances in mass spectrometry.

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

1. Describe the general principles of spectroscopy (UV, IR, NMR & MS) and various chromatographic techniques
2. Solve the structural problems based on UV-Vis, IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR and mass spectral data.

**SUGGESTED READINGS**

1. Banwell, C.N. and McCash, E. M. Fundamentals of Molecular Spectroscopy, 2000, Tata McGraw-Hill, New Delhi.
2. Dyer, J.R. Application of Absorption Spectroscopy of Organic Compounds, 2009, Phi Learning.
3. Kalsi, P.S. Spectroscopy of Organic Compounds, 2004, New Age International Ltd.
4. Kemp, W.Organic spectroscopy, 1991, ELBS London.
5. Khopkar, S.M. Basic Concepts of Analytical Chemistry,2007, New Age International Pvt Ltd.
6. Melinda, J.D. Introduction to solid NMR Spectroscopy, 2010, Wiley India Pvt Ltd

7. Mendham, J., Denney, R.C., Barnes, J. D. and Thomas, M. J. K. Vogel's Textbook of Quantitative Chemical Analysis, 2003, Pearson Education Pvt. Ltd., New Delhi.
8. Pavia, D.L., Lampman, G. M., Kriz, G. S. And Vyavan, J. R. Introduction to Spectroscopy, 4<sup>th</sup> Edition, 2010, Harcourt College, NY.
9. Popov, A.I.; Halenga, K. Modern NMR techniques and their Applications in Chemistry, 1991, Marcel Dekker.
10. Silverstein, R.M., Webster, F. X., Kiemle, D. J. And Bryce, D. L. Spectrometric Identifications of Organic Compounds, 8<sup>th</sup> Edition, 2014, John Wiley.
11. Skoog, D.A., Holler, F.J., and Crouch, S.R., Principles of Instrumental Analysis, 6<sup>th</sup> Edition, 2007 Thomson Learning.
12. Willard, H.H., Merritt Jr. L., Dean, J.A. and Settle, F.A., Instrumental Methods of Analysis, 7<sup>th</sup> edition, 2007, CBS Publishers.
13. Williams, D.H.; Fleming, I. Spectroscopy Methods in Organic Chemistry, 6<sup>th</sup> Edition, 2008, Tata McGraw-Hill Publishing Co. Ltd., New Delhi.

**Course Title: Research Methodology**

**Paper Code: CHL.607**

**Total Lectures: 36**

L	T	P	Credits	Marks
2	0	0	0	50

**Course objective:** To impart knowledge of scientific research tools including search engines, GLP, IPR, library indexing and research writing, which are essential for reporting research work in research laboratories.

**Unit 1** **10 Hrs**

**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.

**Technical writing:** Scientific writing, writing research paper, poster preparation and presentation and dissertation.

**Library:** Classification systems, e-library, reference management, web-based literature search engines

**Unit 2** **10 Hrs**

**Entrepreneurship and business development:** Importance of entrepreneurship and its relevance in career growth, characteristics of entrepreneurs, developing entrepreneurial competencies, types of enterprises and ownership (large, medium SSI, tiny and cottage industries, limited, public limited, private limited, partnership, sole proprietorship), employment, self employment and entrepreneurship, financial management-importance and techniques, financial statements- importance and its interpretation,

**Good Laboratory Practices:** Recent updates on good laboratory practices.

**Unit 3** **16 Hrs**

**Intellectual Property Rights:** Intellectual Property, intellectual property protection (IPP) and intellectual property rights (IPR), WTO (World Trade Organization), WIPO (World Intellectual Property Organization), GATT (General Agreement on Tariff and Trade), TRIPs (Trade Related Intellectual Property Rights), TRIMS (Trade Related Investment Measures) and GATS (General Agreement on Trades in Services), nuts and bolts of patenting, technology development/transfer commercialization related aspects, ethics and values in IP.

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

1. Research writings and would be able to propose his synopsis and dissertation work in the upcoming semester.
2. Present research data at various stages of development.
3. To perform experiments in the laboratory in amicable manner with reporting the critical observation and developing critical thinking.
4. Research ethics and IPR.

**SUGGESTED READINGS**

1. Gupta, S. Research Methodology and Statistical Techniques, 2008, Deep & Deep Publications (p) Ltd. New Delhi.
2. Kothari, C. R. Research methodology(s), 3<sup>rd</sup> Edition, 2014, New Age International (p) Limited. New Delhi
3. Best, J. W. and Khan, J. V. Research in Education, 7<sup>th</sup> edition, 1993, Prentice Hall of India Pvt. Ltd.
4. Wadedhra B.L. Law Relating to Patents, Trademarks, Copyright Design and Geographical Indications. 5<sup>th</sup> Edition, 2014, Universal Law Publishing, New Delhi.
5. Safe science: promoting a culture of safety in academic chemical research; National Academic Press, [website: www.nap.edu].

6. Copyright Protection in India [website: <http://copyright.gov.in>].
7. World Trade Organization [website: [www.wto.org](http://www.wto.org)].

**Course Title: Practical Organic Chemistry-III****Paper Code: CHP.603****Total Contact Hours: 72**

L	T	P	Credits	Marks
0	0	4	2	50

**Course objective:** To provide knowledge of various methodologies for synthesis of target molecules and characterization by spectroscopy techniques.

**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. Exercises of structure elucidation of unknown compounds via combined spectral interpretation of  $^1H$ ,  $^{13}C$  NMR, IR, UV and Mass along with 2-D NMR spectra.****2. Synthesis:** Separation and purification of organic compounds by column chromatography, percentage yield calculation (Any six)

1. Preparation of allylic alcohols via Baylis-Hillman reaction using DABCO as a catalyst under neat condition and their characterization through various spectroscopic techniques.
2. To study Buchwald-Hartwig reaction of aryl halide with an amine using Cu-based catalyst.
3. Synthesis of triazole via reaction of phenylacetylene with azide in water (Huisgen cycloaddition).
4. Synthesis of stilbenes via Heck coupling Strategy.
5. To study decarboxylation of Ferulic acid under microwave irradiation.
6. Regioselective reduction of  $\alpha$ ,  $\beta$  unsaturated carbonyl compound under microwave irradiation.
7. Synthesis of imidazolium and pyridinium based ionic liquids.
8. To study dehydration of benzylic alcohols using imidazolium based ionic liquid.
9. To synthesize 2-phenyl-1,3,4-oxadiazole from benzhydrazide.
10. To synthesize substituted benzodiazepine from chalcone via reflux conditions.
11. To synthesize *p*-nitrobenzaldehyde oxime from *p*-nitrobenzaldehyde.
12. Synthesis of isooxazoline from prior synthesized oxime.
13. Synthesis of benzothiazole starting from 2-aminothiophenol.
14. To study amination of benzothiazole with various amines.
15. To synthesize acylidine analogues of Meldrum acid.

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

1. Drying of various solvents using sodium metal and  $P_2O_5$  and their disposal.
2. Structure elucidation of unknown compounds via interpretation of the spectra (NMR, IR, UV & MS)
3. Various reactions conditions including modern coupling strategies and their implications.

**SUGGESTED READINGS**



1. Harwood, L.M. and Moody, C.J. Experimental Organic Chemistry, 1<sup>st</sup> edition, 1989, Blackwell Scientific Publishers.
2. Vogel, A.I. Textbook of Practical Organic Chemistry, 6<sup>th</sup> edition, 1978, ELBS, Longman Group Ltd.
3. Mann, F.G. and Saunders, B.C. Practical Organic Chemistry, 4<sup>th</sup> edition, New Impression, 1975, Orient Longman Pvt. Ltd.
4. Viswas, A. And Tewari, K.S. A Textbook of Organic Chemistry, 3<sup>rd</sup> edition, 2009 Vikas Publishing House.
5. Leonard, J. and Lygo, B. Advanced Practical Organic Chemistry, 1995, Chapman and Hall,.
6. Armarego, W. L. and Chai, C. Purification of Laboratory Chemicals, 2012, Butterworth-Heinemann.
7. Young, J. A. Improving safety in the chemical laboratory: a practical guide. 2<sup>nd</sup> Edition, 1991, Wiley Publishing.

**Course Title: Practical Physical Chemistry-III****Paper Code: CHP.605****Total Contact Hours: 72**

L	T	P	Credits	Marks
0	0	4	2	50

**Course objective:** To provide training and hand-on experiences of different analytical techniques for chemical analysis and verifications of physical and chemical properties.

**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 CCl<sub>4</sub>/equilibrium constant of tri-iodide formation.
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  $S^{2-}O_8^{2-} + I^- \rightarrow SO_4^{2-} + I_2$  reaction
10. Determination of energy of activation of  $S^{2-}O_8^{2-} + I^- \rightarrow SO_4^{2-} + I_2$  reaction
11. Studies on the effect of variation of ionic strength on the rate of  $S^{2-}O_8^{2-} + I^- \rightarrow SO_4^{2-} + I_2$  reaction
12. Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine clock reaction.

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

1. Experimental techniques for controlling the chemical reactions.
2. Measurement of various physical and chemical properties.
3. Applying related experiments for their research work.

**SUGGESTED READINGS**

1. Nad, A. K., Mahapatra, B. and Ghoshal, A. An Advanced Course in Practical Chemistry, 2014, New Central Book Agency (P) Ltd.
2. Maity S. and Ghosh, N. Physical Chemistry Practical, 2012, New Central Book Agency (P) Ltd.
3. Elias, A. J. Collection of Interesting General Chemistry Experiments, 2008, Universities Press.
4. Khosla, B.D., Garg, V.C., and Gulati A.R., Senior Practical Physical Chemistry, 2007, S. Chand & Sons.
5. Yadav, J.B. Advanced Practical Physical Chemistry, 2008, Krishna Prakashan Media.
6. Das, R.C. and Behra, B. Experimental Physical Chemistry, 1983, Tata McGraw-Hill.
7. James, A.M. and Prichard, F.E. Practical Physical Chemistry, 3<sup>rd</sup> edition, 1974, Longman, Harlow.
8. Ghosh, J.C., Experiments in Physical Chemistry, 1990, Bharati Bhavan.

**Course Title: Inorganic Photochemistry****Paper Code: CHL.608****Total Lectures: 72****Course Objective:** To acquire knowledge of Inorganic photochemistry and photophysical principles, their applications on simple and macromolecules.

L	T	P	Credits	Marks
4	1	0	4	100

**Unit 1****18 Hrs**

**Basics of photochemistry:** Absorption, excitation, laws of photochemistry, quantum yield, lifetime of excited states, Franck-Condon principles, photochemical stages-primary and secondary process; atomic and molecular term symbols, electronic transitions, Jablonski diagram and photophysical processes, radiative transitions, absorption and emission, phosphorescence, intersystem crossing, mechanisms of singlet-triplet conversion (spin-orbit coupling), spin rephasing, spin flip, examples of ISC between states of different configurations, radiative rates, radiationless transitions, internal conversion, energy gap.

**Unit 2****18 Hrs**

**Photochemical Mechanism:** Properties of excited states- structure, dipole moment, acid-base strength, reactivity; 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 3****18 Hrs**

**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 & SET), exciplex formation,

**Redox Processes:** Conditions of the excited states to be useful redox reactants, excited electron transfer, photochemical reactions of Cr, Fe and Ru complexes, role of spin-orbit coupling in the lifetime of the complexes, application of redox process for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light; sensitization and metal complex sensitizers; inorganic photochemistry in biological process and their model studies, solar-energy conservation and storage.

**Unit 4****18 Hrs**

**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.

**Course Outcomes:** The student will have knowledge of

1. Inorganic photochemistry and photophysical principles.
2. Identification and characterization of transient intermediates by ultrafast modern techniques.
3. Theory of photoreaction.
4. Application of photochemistry and photophysical principles on simple and macromolecules.

**SUGGESTED READINGS**

1. Lakowicz, J. R. Principles of Fluorescence Spectroscopy, 3<sup>rd</sup> edition, 2006, Springer.

2. Adamson, A. W. and Fleischauer, P. D. Concepts of Inorganic Photochemistry. 1975, Wiley International.
3. Rohatgi-Mukherjee, K. K. Fundamentals of Photochemistry. 2<sup>nd</sup> Edition, 1986, New Age International.
4. Kryukov, A. I., and S. Yakuchmii. Fundamentals of Photochemistry of Coordination Compounds, 1990.
5. Kavarnos, G. J. Fundamentals of Photoinduced Electron Transfer, 1993, Wiley-VCH publishers Inc., New York.
6. Valeur, B. Molecular Fluorescence: Principles and Applications, 2002, Wiley-VCH Verlag GmbH, Weinheim.
7. Turro, N. J. Ramamurthy, V. and Scaiano, J. C. Modern Molecular Photochemistry of Organic Molecules, 2010, University Science, Books, CA.
8. Ninomiya, I. and Naito, T. Photochemical Synthesis, 1989, Academic Press, New York.

**Course Title: Current Trends in Organic Synthesis****Paper Code: CHL.609****Total Lectures: 72****Course Objective:** To update the knowledge in organic chemistry to an advanced level suited for the industrial tailored synthetic approaches

L	T	P	Credits	Marks
4	1	0	4	100

**Unit 1****18 Hrs****Free radical reactions**

Types of free radical reactions, free radical substitution mechanism at an aromatic substrate, neighbouring group assistance, reactivity for aliphatic and aromatic substrates at a bridgehead, reactivity in the attacking radicals, the effect of solvents on reactivity, allylic halogenation (NBS/NCC/NIS), oxidation of aldehydes to carboxylic acids, auto-oxidation. coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction, free radical rearrangement, Hunsdiecker reaction

**Unit 2****18 Hrs**

**Alkylation:** Enolates: 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 3****18 Hrs****Protection and deprotection of various functional groups:**

Protection of alcohols by ether, silyl ethers and ester formations 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 carbonyls by acetal and ketal formation and their deprotection, protection of carboxylic acids by ester formation and their deprotection

**Unit 4****18 Hrs**

**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, BINAL and BINAP assisted reactions. Ugi reaction, Robinson-Gabriel synthesis, Strecker amino acid synthesis Vilsmeier-Haack reaction, Wohl-Ziegler reaction.

**Course Outcome:** The student would acquire the knowledge of

1. Regioselective and enantioselective C-C bond
2. Judicious use of Protection and deprotection based synthesis.
3. Reaction of commercial importance and their control.

**SUGGESTED READINGS**

1. Finar, I.L., Organic Chemistry Vol. 1, 6<sup>th</sup> edition, 2012, Pearson Education, UK.
2. Finar, I.L., Organic Chemistry Vol. 2: Stereochemistry and the Chemistry of Natural Products, 6<sup>th</sup> edition, 2012, Pearson Education, UK.
3. Fleming I. Pericyclic Reactions, 1999, Oxford University Press.
4. Fleming I. Molecular Orbitals and Organic Chemical Reactions, 2011, John Wiley & Sons.

5. Li, J. J. Name Reactions: A collection of Detailed Reaction Mechanism, 5<sup>th</sup> edition, 2014, Springer-Verlag.
6. Kalsi, P.S. Organic Reactions and Their Mechanisms, 3<sup>rd</sup> edition, 2010, New Age International Pub., New Delhi.
7. Kalsi, P.S. Stereochemistry: Conformation and Mechanism, 6<sup>th</sup> edition, 2008, New Age International (p) Ltd., New Delhi.
8. Lowry, T. H. and Richardson K. S. Mechanism and Theory in Organic Chemistry, 3<sup>rd</sup> edition, 1998, Addison-Wesley Longman Inc., New York.
9. McMurry J. Organic Chemistry, 8<sup>th</sup> edition, 2011 Asian Book Pvt. Ltd, New Delhi
10. Morrison, R.T. and Boyd, R.N. Organic Chemistry, 6<sup>th</sup> edition, 2011, Prentice- Hall of India, New Delhi.
11. Mukherjee, S.M. and Singh, S.P. Reaction Mechanism in Organic Chemistry. 3<sup>rd</sup> edition, 2009, Macmillan India Ltd., New Delhi.
12. Bruckner, R. Advanced organic chemistry: Reaction Mechanism, 2001, Academic Press.
13. Smith, M. B. March's advanced organic chemistry: reactions, mechanisms, and structure, 7<sup>th</sup> Edition, 2013, John Wiley & Sons.
14. Solomon, T.W.G, Fryhle, C.B. and Snyder, S. A. Organic Chemistry. 11<sup>th</sup> edition, 2013, John Wiley and Sons, Inc.
15. Sykes, P. A Guide Book to Mechanism in Organic Chemistry, 6<sup>th</sup> edition, 1997, Prentice Hall.
16. Carruthers, W. Some Modern Methods of Organic Synthesis, 4<sup>th</sup> edition, 2004, Cambridge Uni. Press, UK.

**Course Title: Supramolecular Chemistry**

L	T	P	Credits	Marks
4	1	0	4	100

**Paper Code: CHL.610****Total Lectures: 72**

**Course Objective:** To impart knowledge of molecular interactions apart from bonding. Use of such interactions in template host and their designing for complimentary target guest and devising supramolecules which could be applied as organic materials, sensors, and devices.

**Unit 1** **18 Hrs**

**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- $\pi$ ,  $\pi$  -  $\pi$  and vanderwaal 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.

**Unit 2** **18 Hrs**

**Cation and Anion Binding:** 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 and template effects, soft ligands, carbon donor and  $\pi$ - acid ligands, siderophores.

biological anion receptors, concepts on anion host design, from cation to anion hosts- a simple change in pH, guanidinium- based receptors, neutral receptors, organometallic receptors, coordination interactions.

**Unit 3** **18 Hrs**

**Molecular self-assembly:** Supramolecular polymers: definition, types of intermolecular interactions and their energetics. self-assembly molecules: design, synthesis and properties of the molecules, self-assembly by H-bonding, catenanes, rotaxanes, molecular knot bromenean rings dendrimers and supramolecular gels. relevance of supramolecular chemistry to mimic biological system. thermodynamics and kinetic stability of supramolecular systems and their applications. fullness as hosts or guests and as superconducting intercalation compounds and their applications.

**Unit 4** **18 Hrs**

**Supramolecular and Molecular Devices:** Supramolecular photochemistry, molecular electronic devices: molecular electronic devices, molecular wires, molecular rectifiers, molecular switches and molecular logic gates, machines based on catenanes and rotaxanes organics for photonics and electronics.

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

1. Various supramolecular aspects of interaction between two chemical systems.
2. Devising supramolecular systems based on complementarity and preorganizational requirements of host.

**SUGGESTED READINGS**

1. Steed J.W and Atwood, J.L Supramolecular chemistry, 2<sup>nd</sup> Edition, John Wiley & Sons, Ltd. New York.
2. Lehn, J. M., Supramolecular Chemistry-Concepts and Perspectives, Wiley –VCH (1995).
3. P.D., Beer, Gale, P. A., and Smith, D. K., Supramolecular Chemistry, 1999, Oxford University Press.
4. Martin, N. and Nierengarten J.-F. Supramolecular Chemistry of Fullerenes and Carbon Nanotubes, 2012, Wiley-VCH.

5. Vicens, J. and Harrowfield J. Calixarenes in the Nanoworld, 2007, Springer.
6. Schalley, C. A. Analytical Methods in Supramolecular Chemistry, 2nd Edition, Volume 1 & 2, 2012, Wiley-VCH



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

**Paper Code: CHL.621**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Course objective:** To impart knowledge of polymers, solid state chemistry and nanomaterials.

**Unit 1** **18 Hrs**

**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 2** **18 Hrs**

**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.

**Conducting Polymers:** Synthesis of conducting polymers, preparation of conducting polymers for various devices like electronic devices, chemical sensors, solar cells, light emitting devices, biomedical devices

**Unit 3** **18 Hrs**

**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.

**Unit 4** **18 Hrs**

**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.

**Course Outcome:** After completion of this course, the students will acquire knowledge of

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

### **SUGGESTED READINGS**

1. Gowariker, V. R., Viswanathan, N. V. and SreedharJ. Polymer Science, 1<sup>st</sup> Edition, 1986, New Age International Pvt. Ltd., New Delhi.
2. Odian, G., Principles of Polymerization, 4<sup>th</sup> Edition, 2007, John Wiley & Sons.
3. Peacock, A. and Calhoun, A. Polymer Chemistry-Properties and Applications, 2006, Carl Hanser Verlag GmbH & Company KG.
4. Chandra, R. and Adab, A., Rubber and Plastic Waste, 1994, CBS Publishers & Distributors, New Delhi.
5. Bahadur, P., and Sastry, N. V., Principles of Polymerisation, 2<sup>nd</sup> Edition, 2006, Narosa Publishing House, New Delhi .
6. Keer, H.V. Principle of the Solid State, 1993, New Age International.
7. Ashcroft, N.W. and Mermin, N.D. Solid State Physics, 1976, Saunders College.
8. Callister, W.D. and Rethwisch, D. G. Material Science and Engineering, An Introduction, 9<sup>th</sup> Edition, 2014, Willey.
9. Anderson, J.C. Leaver, K.D. Alexander J.M. and Rawlings, R.D. Material Science, 5<sup>th</sup> Edition, 2003, Nelson and Thornes.

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

**Paper Code: CHL.622**

**Total Lectures: 72**

**Course objective:** To provide knowledge of structure, function, and physicochemical properties of biomolecules.

L	T	P	Credits	Marks
4	1	0	4	100

### Unit 1

18 Hrs

#### Inorganic Chemistry of Enzymes - I

Introduction, energy sources for life, non-photosynthetic processes, metalloporphyrins, cytochromes, biochemistry of iron, iron storage and transport, ferritin transferring, bacterial iron transport, hemoglobin and myoglobin, nature of heme-dioxygen binding, model systems, cooperativity in hemoglobin, physiology of myoglobin and hemoglobin, structure and function of hemoglobin. Other iron-prophyrin biomolecules, structure and function of hemoglobin. Other iron-porphyrin biomolecules, peroxidases and catalases, cytochrome P450 enzymes, other natural oxygen carriers, hemerythrins, electron transfer.

### Unit 2

18Hrs

#### Inorganic Chemistry of Enzymes - II

Respiration and photosynthesis; ferridoxins, and subredonim carboxypeptidase, carbonicanhydrase, metallothioneins. Bblue copper proteins, superoxide dismutase hemocyanines photosynthesis, chlorophyll and photosynthetic reaction center.

**Enzymes:** Structure and function, inhibition and poisoning vitamin B<sub>12</sub> and B<sub>12</sub> coenzymes metallothioneins, nitrogen fixation, in-vitro and in-vivo nitrogen fixation, bio-inorganic chemistry of Mo and W, nitrogenases: other elements V, Cr, Ni (essential and trace elements in biological systems).

### Unit 3

18 Hrs

#### Metal Ions in Biological Systems

Metal complexes of polynucleotides, nucleosides and nucleic acids (DNA & RNA). template temperature, stability of DNA. role of metal ions in replication and transcription process of nucleic acids. biochemistry of dioxygen, bioinorganic chips and biosensors. biochemistry of calcium as hormonal messenger, muscle contraction blood clotting, neurotransmitter, calcification reclaiming of barren land. metals in the regulation of biochemical events. transport and storage of metal ions *in vivo*. metal complexes as probes of structure and reactivity with metal substitution.

### Unit 4

18 Hrs

#### Biophysical Chemistry

Principles of biophysical chemistry (pH, buffer, reaction kinetics, thermodynamics, colligative properties), structure and physical properties of amino acids, 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), mechanisms of protein folding, thermodynamics of protein folding by spectroscopic and calorimetric methods, ultrafast folding dynamics study by laser flash photolysis, protein conformational study by NMR and fluorescence spectroscopy, measurement of hydrodynamic radii by dynamic light scatter

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

1. Structure and biological functions of proteins and enzymes.

2. The role of metals in biology
3. Factors that govern the thermodynamic stability, folding, and dynamics of proteins.
4. Kinetics, thermodynamics, and mechanism of protein folding.

#### **SUGGESTED READINGS**

1. Huheey, J. E., Keiter, E. A. and Keiter, R.L. Inorganic Chemistry Principles of Structure and Reactivity, 4<sup>th</sup> edition, 2006, Haper Collins.
2. Douglas, B., McDaniel, D. and Alexander, J. Concepts and Models of Inorganic Chemistry, 3<sup>rd</sup> edition, 2006, John Wiley and Sons.
3. Cotton, F.A. and Wilkinson, G. Advanced Inorganic Chemistry: A Comprehensive Text, John Wiley, 5th edition.
4. Elschenbroich, Ch. and Salzer, A. Organometallics. A Concise Introduction, 2<sup>nd</sup> edition, 1992, Wiley-VCH.
5. Atkins, P., Overton, T., Rourke, J., Weller, J. and Armstrong, F. Shriver and Atkin's Inorganic Chemistry, 5<sup>th</sup> edition, 2010, Oxford University Press.
6. Cowan, J.A. Inorganic Biochemistry: An Introduction, 2nd edition, 1997, Wiley – VCH.
7. Lippard, S. J. Progress in Inorganic Chemistry, Vols. 18, 1991, Wiley-Interscience.
8. Lippard, S. J. Progress in Inorganic Chemistry, Vols. 38, 1991, Wiley-Interscience.
9. Lesk, A.M., Introduction to Protein Science: Architecture, Function, and Genomics, 2<sup>nd</sup> edition, 2010, Oxford University Press.
10. Cantor, C.R. and Schimmel, P.R., Biophysical Chemistry, 1980, Freeman.
11. Van Holde, K.E., Johnson, W.C. and Ho, P.S., Principles of Physical Biochemistry, 2<sup>nd</sup> Edition, 2006, Pearson Education.
12. Harding, S.E. and Chowdhry, B. Z. Protein-Ligand Interactions, 2001, Oxford University Press.

**Course Title: Advanced Organic Synthesis**

**Paper Code: CHL.623**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Course objective:** To impart knowledge of various important topics in organic synthesis such as asymmetric synthesis, reagents including organometallic reagents and some important reactions of ylides.

**Unit 1 14 Hrs**

**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 2 18 Hrs**

**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: Peterson's olefin synthesis. Sulphur Ylides; stabilized and non-stabilized ylides: thermodynamically and kinetically controlled reactions with carbonyl compounds, regio- and stereo-selective reactions, Staudinger Reaction, Mitsunobu reaction.

**Unit 3 20 Hrs**

**Organometallic compounds**

Organoboranes: Preparation of organoboranes viz hydroboration with  $\text{BH}_3\text{-THF}$ , dicyclohexyl borane, disiamyl borane, hexyl borane, 9-BBN and disopinocampheyl borane, functional group transformations of organo boranes: oxidation, protonolysis and rearrangements. formation of carbon-carbon-bonds viz organo boranes carbonylation.

Grignard reagents, organolithium, organozinc, organocadmium and organocopper compounds, organosilicon compounds for organic synthesis, organopalladium and organostannous (applications in coupling reactions).

**Unit 4 20 Hrs**

**Reagents in organic synthesis:** Gilman's reagent, Lithiumdiisopropylamide(LDA), 1,3-Dithiane (Umpolung reagent), Trimethylsilyliodide, Baker's yeast, Prevost Hydroxylation, Wilkinson's catalyst, Phase transfer catalysts: quaternary ammonium and Phosphonium salts, Crown ethers, Merrifield resin, Fenton's reagents, Ziegler-Natta catalyst, Lawesson reagents, K-selectride and L-selectride, Sodium cyanoborohydride, IBX, Sodium triacetoxyborohydride, Fetizon reagent, Dioxiranes, Ceric ammonium nitrate, Tebbe reagent, Corey-Nicolaou reagent, Mosher's reagent, use of Os, Ru, and Tl reagents.

**Course Outcomes:** The students will acquire knowledge of

- Asymmetric synthesis and chiral resolution.
- Various reagents including organometallic compounds, experimental conditions and their applications in organic synthesis/industry.
- Some important reactions utilizing phosphorus and sulphur ylides.

**SUGGESTED READINGS**

1. Claydon, J., Gleeves, N., Warren, S. and Wothers, P. Organic chemistry, 2001, Oxford University Press, UK.
2. Fieser and Fieser, Reagents for organic synthesis, Vol 1-26, 3<sup>rd</sup> edition, 2011, Wiley Interscience.

3. Finar, I.L. Organic Chemistry, 6<sup>th</sup> edition, 2012, Pearson Education, UK.
4. Li, J.J. Name Reactions: A Collection of Detailed Reaction Mechanism 4<sup>th</sup> edition, 2009 Springer.
5. Smith, M. B. March's advanced organic chemistry: reactions, mechanisms, and structure. 7<sup>th</sup> Edition, 2013, John Wiley & Sons.
6. Reich, H.J. and Rigby, M. Handbook of Reagents for Organic Synthesis Acidic and Basic Reagents Vol. IV, 1999, Wiley-Interscience.
7. Warren, S. Organic synthesis: The Synthons Approach. 2010, John Wiley & Sons, New York,
8. Warren, S. and Wyatt, P. Designing Organic synthesis: A Disconnection Approach. 2<sup>nd</sup> Edition, 2010, John Wiley & Sons, New York.
9. Corey E.J. and Cheng, X.-M. The Logic of Chemical Synthesis, 1989, John Wiley & Sons.
10. Fuhrhop J.-H. and Penzlin, G. Organic Synthesis: Concepts methods, Starting Materials, 2<sup>nd</sup> edition, 1994, Verlag chemie.
11. Davies S. G., Organotransition Metal Chemistry: Application to Organic Synthesis, 1994, Pergamon Press.
12. Morrison J. D. (eds) Asymmetric Synthesis, Vol. 1 to 5, 1992, Academic Press.
13. Aitken R.A. and Kilenyi S.N., Asymmetric Synthesis, 1992, Springer Publishers.
14. Proctor G. Asymmetric Synthesis, 1996, Academic Press.

**Course Title: Material Chemistry**

**Paper Code: CHL.624**

**Total Lectures: 72**

**Course objective:** To impart knowledge of materials, their characteristics and physical functions

L	T	P	Credits	Marks
4	1	0	4	100

**Unit 1: 18 Hrs**

**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 2: 24 Hrs**

Mesomorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic - nematic transition and clearing temperature -homeotropic, planar and schlieren 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 3: 12 Hrs**

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 (phenylene vinylene)s, oligo( phenylene ethynylene)s, oligo (eneyne)s, oligo(thiophene vinylene), oligo (thiophene ethynylene) etc. and their applications.

**Unit 4: 18 Hrs**

**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.

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

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

## **SUGGESTED READINGS**

1. Ashcroft, N.W. and Mermin, N.D. Solid State Physics, 1976, Saunders College.
2. Callister, W.D. and Rethwisch, D. G. Material Science and Engineering, An Introduction, 9<sup>th</sup> Edition, 2014, Willey.
3. Anderson, J.C. Leaver, K.D. Alexander J.M. and Rawlings, R.D. Material Science, 5<sup>th</sup> Edition, 2003, Nelson and Thornes.
4. Keer, H.V. Principle of the Solid State, 1993, New Age International.



**Course Title: Chemistry of Natural Products**

**Paper Code: CHL.625**

**Total Lectures: 72**

**Course Objective:** The course provides a brief introduction, classification, occurrence and biosynthesis of various natural products.

L	T	P	Credits	Marks
4	1	0	4	100

**Unit 1** **18 Hrs**

**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 2** **18 Hrs**

**Alkaloids:** Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, Nicotine and Morphine.

**Unit 3** **18 Hrs**

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

**Unit 4** **18 Hrs**

**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

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

1. Become familiar with various types of natural products and their importance.
2. Identify various types of natural products including their properties, occurrence, structure and biosynthesis.

**SUGGESTED READINGS**

1. Bhat, S.V., Nagasampagi, B.A., Meenakshi, S. Natural Product Chemistry & Applications, 2009, Narosa Publishing House, New Delhi.
2. Bhat, S.V., Nagasampagi, B.A., Sivakumar, M. Chemistry of Natural Products 2005, Narosa Publishing House, New Delhi.
3. Brahamchari, G. Natural Product: Chemistry, Biochemistry and Pharmacology 2009, Narosa Publishing House, New Delhi.
4. Cseke, L.J. Natural Products from plants 2<sup>nd</sup> edition, 2009, CRC Press, Taylor and Francis US.
5. Dewick, P.M. Medicinal Natural Products: A Biosynthetic Approach 3<sup>rd</sup> edition, 2009, Willey & Sons, UK.
6. Finar, I.L. Organic Chemistry: Stereochemistry and the Chemistry of Natural Products. 6<sup>th</sup> edition, 2006, Dorling Kindersley Pvt. Ltd., India.
7. Peterson, F. and Amstutz, R. Natural Compounds as drugs, 2008, Birkhauser Verlag.
8. Thomson, R.H. The Chemistry of Natural Products, 1<sup>st</sup> edition, 2008, Springer,.

**Course Title: Organotransition Metal Chemistry**

**Paper Code: CHL.626**

**Total Lectures: 72**

**Course Objective:** The course provides advanced knowledge of organotransition metal chemistry

L	T	P	Credits	Marks
4	1	0	4	100

### Unit 1

18 Hrs

#### Compounds of Transition Metal-Carbon Multiple Bonds

Alkylidenes, alkylidynes, low valent carbenes and carbynes-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reaction on the ligands, role in organic synthesis

### Unit 2

18 Hrs

#### Transition Metal Complexes

Transition metal complexes with 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, metallocenes.

### Unit 3

18 Hrs

#### Alkyls and Aryls of Transition Metals

Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis.

#### Fluxional organometallic compounds

Fluxionality and dynamic equilibria in compounds such as  $\eta^2$  olefin,  $\eta^2$  allyl and dienyl complexes.

### Unit 4

18 Hrs

#### 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) oxopalladation reactions, activation of C-H bond.

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

1. Transition metal complexes and compounds of transition metal-carbon multiple bonds
2. Alkyls and aryls of transition metals and fluxional organometallic compounds
3. Homogeneous catalysis and their applications.

### SUGGESTED READINGS

1. Collman, J.P.; Norton, J.R.; Hegsdus, L.S.; Finke, R.G. Principles and Application of Organotransition Metal Chemistry, 1987, University Science Books.
2. Crabtree, R.G. The Organometallic Chemistry of the Transition Metals, 5<sup>th</sup> edition, 2011, John Wiley.
3. Mehrotra R. C. and Singh, A. Organometallic Chemistry, 2<sup>nd</sup> edition, 2005, New Age International.
4. Cotton, F.A. and Wilkinson, G. Advanced Inorganic Chemistry, 6<sup>th</sup> edition, 1999, John Wiley.
5. Pearson, A.J. Metallo-Organic Chemistry, 1985, Wiley.

## Interdisciplinary Courses Offered by Centre for Chemical Sciences

ID Courses offered by the faculty of Centre for Chemical Sciences (For students of other Centers)											
1	CHL.509	Basics perspective in Inorganic Chemistry	2	-	-	2	10	15	15	10	50
2	CHL.510	Introduction to Green Chemistry and Sustainability	2	-	-	2	10	15	15	10	50
3	CHL.511	Chemistry of Nanomaterials and Fabrication	2	-	-	2	10	15	15	10	50

**Course Title: Basic Perspectives in Inorganic Chemistry****Paper Code: CHL.509****Total Lectures: 36**

L	T	P	Credits	Marks
2	0	0	2	100

**Course Objective:** To introduce the knowledge of d-block elements, coordination chemistry, ions role in biology, metals in aqueous environment, and hydrogen energy.

**Unit 1** **8 Hrs**

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

**Unit 2** **10 Hrs**

Ions role in bioscience: ionophores, popyrin and other tetrapyrrollic macromolecules, coenzymes, neurotransmitters, metal binding to dna.

**Unit 3** **10 Hrs**

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

**Unit 4** **8 Hrs**

**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.

**Course Outcome:** The completion of this course will enable the students to acquire knowledge of

1. The coordination chemistry of d-group elements and coordination of ions within living organisms.
2. Environmental chemistry and metal hydrides as hydrogen energy source.

**SUGGESTED READINGS**

1. Cotton, F.A.; Wilkinson Advanced Inorganic Chemistry, 6th edition, 2007, John Wiley & Sons.
2. Huheey, J. E. Inorganic Chemistry: Principles of Structure and Reactivity, 4<sup>th</sup> edition, 2006, Dorling Kindersley (India) Pvt. Ltd.
3. Greenwood, N.N. and Earnshaw, A. Chemistry of the Elements, 2<sup>nd</sup> edition, 2005 (reprinted), Butterworth-Heinemann, A division of Read Educational & Professional Publishing Ltd.
4. Lippard, S.J. and Berg, J.M., Principles of Bioinorganic Chemistry. 1994, University Science Books.
5. Van-Loon G.W. and Duffy S.J. Environmental Chemistry: A Global Perspective, 3<sup>rd</sup> Edition, 2011, Oxford University Press.
6. Rao C.S. Environmental Pollution Control Engineering, 2<sup>nd</sup> Edition, 2006, New Age International Publishers, New Delhi,
7. Peruzzini, M. and Poli, R. Recent Advances in Hydride Chemistry, 2005, Elsevier Science B.V., Amsterdam.

**Course Title: Introduction to Green Chemistry and Sustainability****Paper Code: CHL.510****Total Lectures: 36**

L	T	P	Credits	Marks
2	0	0	2	100

**Course objective:** To introduce basic concepts of green chemistry and their importance for sustainable development.**Unit 1****10 Hrs****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 2****14 Hrs****Emerging non-conventional techniques:**

Microwave heating as energy efficient source, sono-chemistry and green chemistry, ionic liquids: use of ionic liquids as solvent as well as catalyst, recyclability of ionic liquids. solvent free conditions.

**Unit 3****12 Hrs****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.

**Course Outcome:** The students will be acquainted with

1. Modern concepts and tools of green chemistry and their importance in sustainable development.
2. Utilization of abundantly available precursors for the production of value added chemicals.

**SUGGESTED READINGS**

1. Anastas, P.T. and Warner J. C. Green chemistry, Theory and Practical. 1<sup>st</sup> edition, 2000, Oxford University Press, US.
  2. Ahluwalia, V.K and Kidwai, M. New Trends in Green Chemistry, 2004, Springer.
  3. Malhotra, S. V. Ionic Liquids in Organic Synthesis, 2007, Oxford University Press, US.
  4. Ahluwalia, V.K.Green Chemistry: Greener Alternatives to Synthetic Organic Transformations, 2011, Alpha Science International Limited.
  5. Klass, D. Biomass for Renewable Energy, Fuels, and Chemicals, Elsevier, 1998
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**Course Title: Chemistry of Nanomaterials and Fabrication**

**Paper Code: CHL.511**

**Total Lectures: 36**

L	T	P	Credits	Marks
2	0	0	2	100

**Course objective:** To impart the basic and recent knowledge of nanomaterials regarding their fabrication, characterization and applications.

### Unit 1

6 Hrs

#### 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 2

10 Hrs

#### 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 3

10 Hrs

#### Nanomaterials and properties:

Influence of nucleation rate on the size of the crystals- macroscopic to microscopic crystals and nanocrystals - 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 4

10 Hrs

#### 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.

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

1. Nanotechnology, fabrication and characterization of nanomaterials, properties and applications of nanomaterials.

### SUGGESTED READINGS

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