

**Centre for Chemical Sciences**  
M.Sc. in Chemical Sciences  
Syllabus

**SEMESTER 1**

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	Weightage				E
								A	B	C	D	
1	CHM.501	Computer Applications	FC	2	1	0	2	10	15	15	10	50
2	CHM.502	Inorganic Chemistry-1	CC	4	1		4	25	25	25	25	100
3	CHM.503	Organic Chemistry-1	CC	4	1		4	25	25	25	25	100
4	CHM.504	Physical Chemistry-I	CC	4	1		4	25	25	25	25	100
5	CHM.505	Spectral Analysis	EC	4	1		4	25	25	25	25	100
6	CHM.506	Organic Chemistry-Practical	CC	-	-	4	2	-	-	-	-	50
7	CHM.507	Inorganic Chemistry-Practical	CC	-	-	4	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>20</b>		<b>8</b>	<b>24</b>					<b>600</b>

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

**A:** Continuous Assessment: Subjective by enlarge

**B:** Mid-Term Test-1: Based on Objective Type & Subjective Type Test

**C:** Mid-Term Test-2: Based on Objective Type & Subjective Type Test

**D:** End-Term Exam (Final): Based on Objective Type Tests

**E:** Total Marks

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

**Course Title: Computer Applications**  
**Paper Code: CHM.501**  
**Total Lectures: 54**

L	T	P	Credits	Marks
36	1	0	2	50

### Unit 1

**Fundamentals of computers:** Parts of computers, Hardware, BIOS, Operating systems, Binary system, Logic gates and Boolean algebra.

**Application software:** Spreadsheet applications, Word-processing applications, Presentation applications, Internet browsers, Reference Management, and Image processing applications.

### Unit 2

**Computer language:** Basic DOS commands, AutoHotKey scripting language, HTML and basic structure of a webpage, Designing websites.

**World Wide Web:** Origin and concepts, Latency and bandwidth, Searching the internet, Advanced web-search using Boolean logic, Cloud computing.

### ESSENTIAL BOOKS

1. Gookin, D. (2007). *MS Word 2007 for Dummies*. Wiley.
  2. Harvey, G. (2007). *MS Excel 2007 for Dummies*. Wiley.
  3. Johnson, S. (2009). *Windows 7 on demand*. Perspiration Inc.
  4. Norman, G. and Streiner, D. (3<sup>rd</sup> edn) (2008). *Biostatistics: The Bare Essentials*. Decker Inc., Canada.
  5. Sokal, R.R. and Rohlf, F.J. (1994). *Biometry: The Principles and Practices of Statistics in Biological Research*, W.H. Freeman and Company, New York.
- Thurrott, P. and Rivera, R. (2009). *Windows 7 Secrets*. Wiley

**Course Title: Inorganic Chemistry-I**  
**Paper Code: CHM.502**  
**Total Lectures: 72**

L	T	P	Credits	Marks
72	1	0	4	100

**Unit 1** **12 Hours**

**Metal-Ligand Equilibria in Solution**

Stepwise and overall formation constant and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH spectrophotometry.

**Unit 2** **20 Hours**

**Symmetry Elements and Molecular Orbital Theory**

Symmetry elements, symmetry operations and their matrix representation, group postulates and types, multiplication tables, point group determination, 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, MOEL diagrams for octahedral tetrahedral and square planar complexes showing  $\sigma$  and  $\pi$  bonding in transition metal complexes.

**Unit 3** **20 Hours**

**Crystal Fields Splitting**

Spin-spin, orbital-orbital and spin orbital coupling, LS and jj coupling schemes, determination of all the spectroscopic terms of pn, dn 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 d2 configuration in octahedral and tetrahedral crystal fields (using group theory), construction of the correlation energy level diagrams of d2 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 Centro symmetric and non-centro symmetric 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.

**Unit 4** **20 Hours**

**Electronic Spectra of Transition Metal Complexes**

Variation of the Racah parameter, nephelauxetic effect -central field covalency, symmetry restricted covalency, differential radial expansion, spectrochemical series, band intensities, factors influencing band widths, 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 statesmixing, 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.

#### **ESSENTIAL BOOKS:**

1. Cotton, F.A.; Wilkinson *Advanced Inorganic Chemistry*, 6th edition, John Wiley & Sons, 1999.
2. Huheey, James E. *Inorganic Chemistry: Principles of Structure and Reactivity*, 4<sup>th</sup> edition, Harper Collins College Publishers, 1993.
3. Greenwood, N.N. and Earnshaw, A. *Chemistry of the Elements*, 2nd edition, Butterworth-Heinemann, A division of Read Educational & Professional Publishing Ltd., 2001.
4. Lever, A.B.P. *Inorganic Electronic Spectroscopy*, 2nd edition, Elsevier Science Publishers B.V., 1984.
5. Carlin, Richard L. and Duyneveldt, A.J. Van *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*, Pearson Education, 3rd edition
7. Figgis, B.N. *Introduction to Ligand Field*, Wiley Eastern.
8. Drago, R.S. *Physical Methods in Chemistry*, W.B. Saunders Company.
9. Shriver, D.F.; Atkins, P.W. *Inorganic Chemistry*, 1st edition, Oxford University Press, 2006.
10. Earnshaw, A. *Introduction to Magnetochemistry*, Academic Press, 1968.
11. Dutta, R.L.; Syanal, A. *Elements of Magneto chemistry*, 2nd edition, Affiliated East West Press, 1993.
12. Drago, Russell S. *Physical Methods for Chemists*, 2nd edition, Saunders College Publishing, 1992.

**Course Title: Organic Chemistry-I**

**Paper Code: CHM.503**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Unit 1**

**22 Hours**

**Stereochemistry:** IUPAC nomenclature of organic molecules, Elements of symmetry, chirality, Projection formulae [Fly wedge, 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, DL and RS 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, geometrical isomerism, *cis-trans* and E-Z conventions, methods of inter-conversion of E and Z isomers, determination of configuration by physical and chemical methods.

**Unit 2**

**18 Hours**

**Aliphatic nucleophilic substitution reaction:** The SN<sub>2</sub>, SN<sub>1</sub>, mixed SN<sub>1</sub> and SN<sub>2</sub> and SET mechanism, The S<sub>N</sub>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 SN<sub>1</sub> and SN<sub>2</sub> mechanism.

**Aromatic nucleophilic substitution:** The S<sub>N</sub>Ar, benzyne and SN<sub>1</sub> mechanism, reactivity effect of substrate structure, leaving group and attacking nucleophile.

**Aliphatic electrophilic substitution:** Bimolecular mechanisms SE<sub>2</sub> and SE<sub>1</sub> mechanism, electrophilic substitution accompanied by double bond shifts, effect of substrates, leaving groups and the solvent polarity on the reactivity.

**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, Vilsmeier reaction, Gatterman-Koch reaction.

**Unit 3**

**16 Hours**

**Elimination reactions:** The E<sub>2</sub>, E<sub>1</sub> and E<sub>1</sub>cB mechanisms and their spectrum, orientation of the double bond, reactivity 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, Regio- and

chemoselectivity, orientation and reactivity, hydroboration, alkylation, epoxidation and hydroxylation, addition of halogen polar reagents to alkenes.

#### Unit 4

16 Hours

**Addition to carbon-hetero multiple bonds:** Reactivity of carbonyl group, homologation and dehomologation of carbonyl compounds, nucleophilic addition of hetero-atoms (N,O,S), conjugate addition reactions, acylation of carbonyl carbon, carbonyl cyclizations and cleavages, carboxylic acids and derivatives, decarboxylation reactions, addition of Grignard, 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.

#### ESSENTIAL BOOKS:

1. Finar, I.L., (2003). *Organic Chemistry Vol. 1*. Pearson Education, 4<sup>th</sup> edition.
2. Mc Murry J., *Organic Chemistry*, Asian Book Pvt. Ltd, 8<sup>th</sup> edition, New Delhi
3. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
4. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., 4<sup>th</sup> edition, New Delhi-110002.
5. Bansal, R. K., (2010). *A text book of Organic Chemistry*, New Age International (P) Ltd., 5<sup>th</sup> edition, New Delhi.
6. Bansal R.K., (2010). *Organic Reaction Mechanism*, New Age International (P) Ltd., New Delhi.
7. Kalsi, P.S., (2010). *Organic Reactions and Their Mechanisms*. New Age International Pub., 3<sup>rd</sup> edition, New Delhi.
8. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd. New Delhi.
9. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3<sup>rd</sup> edition, New York.
10. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, 6<sup>th</sup> edition, New Delhi.
11. Mukherjee, S.M. Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd., 3<sup>rd</sup> edition, New Delhi.
12. Robert and Casereo, (1977). *Basic principle of Organic Chemistry*, Addison-Wesley, 2<sup>nd</sup> edition.
13. Solomn, C.W.G, Fryble, C.B. (2009). *Organic Chemistry*. John Wiley and Sons, Inc., 10<sup>th</sup> edition.
14. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, 6<sup>th</sup> edition.
15. Eliel, E. L., & Wilen, S. H. (2008). *Stereochemistry of organic compounds*. John Wiley & Sons.

**Course Title: Physical Chemistry-I**

**Paper Code: CHM.504**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

### Unit 1

**18 Hours**

**Surface Chemistry and Catalysis:** Bimolecular surface reactions-reaction between a gas molecule and adsorbed molecule, reaction between two adsorbed molecules, inhibition and activation energy of such reactions. Catalytic activity at surfaces, transition state theory of surface reactions: rates of chemisorption and desorption, unimolecular and bimolecular surface reaction, comparison of homogeneous and heterogeneous reaction rates, surface heterogeneity, lateral interaction. Adsorption of solids, Gibbs adsorption isotherm, BET adsorption isotherm: estimation of surface area of solids.

### Unit 2

**18 Hours**

**Electrochemistry:** Nernst equation, redox systems, electrochemical cells; Debye-Huckel theory; electrolytic conductance–Kohlrausch’s law and its applications; ionic equilibria; conductometric and potentiometric titrations.

**Solid State:** Crystal structures; Bragg’s law and applications; band structure of solids.

### Unit 3

**16 Hours**

**Chemical Kinetics:** Empirical rate laws and temperature dependence; complex reactions; steady state approximation; determination of reaction mechanisms; collision and transition state theories of rate constants; unimolecular reactions; enzyme kinetics; homogeneous catalysis; photochemical reactions.

### Unit 4

**20 Hours**

**Polymer Chemistry:** Classification of polymers, kinetics of polymerizations, Molecular weight, molecular weight distribution and its control in polymerization. Copolymerization, polymerization techniques and control of polymer structure and properties and its applications.

**Nuclear Chemistry:** Classification of nuclides, Nuclear stability, Atomic energy, Types of nuclear reactions–fission and fusion, Conservation in nuclear reactions-linear momentum and mass-energy, Reaction cross-section, Bohr’s compound nucleus theory of nuclear reaction.

### ESSENTIAL BOOKS:

1. Physical Chemistry, G. M. Barrow, TATA MCGRAW-HILL, 2007.
2. Text Book of Physical Chemistry, K. L. Kapoor, MACMILLAN, 2006.
3. Physical Chemistry, A. W. Atkins, W. H. Freeman, and Company, 1997.
4. Physical Chemistry: A Molecular Approach, D. A. McQuarrie, and J. D. Simon, Viva Books, 2011.
5. Kinetics and Mechanism, J. W. Moore, and R. G. Pearson, John Wiley and Sons, 1981.
6. Physical Chemistry, R. J. Silbey, R. A. Alberty, and M. G. Bawendi, Wiley-Interscience Publication, 2013.
7. Physical Chemistry, T. Engel, and P. Reid, Prentice-Hall, 2012.

**Course Title: Spectral Analysis**

**Paper Code: CHM.505**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

### **Unit 1**

**18 Hours**

**UV-Visible spectroscopy:** Principle of UV-Visible Spectroscopy, Chromophores and their interaction with UV-visible radiation and their utilization in structural, qualitative and quantitative analysis of drug molecules. Woodward-Fieser rule, solvent effects, stereochemical effect.

**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**

**18 Hours**

**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**

**18 Hours**

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 enhanced (NOE), <sup>13</sup>C NMR spectra, their interpretation and application. APT and 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, DEPT and 2D INADEQUATE experiments and their application, Solid-state NMR.

### **Unit 4**

**18 Hours**

**Mass spectrometry:** Basic principles and brief outline of instrumentation, Ion formation, molecular ion, metastable ion, Mc Lafferty 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.

### **ESSENTIAL BOOKS:**

1. Banwell, C.N.; McCash, E. M. (2000). *Fundamentals of molecular spectroscopy*, Tata McGraw-Hill, New Delhi.
2. Dyer, J.R. (2009). *Application of Absorption Spectroscopy of Organic Compounds*, Publisher: Phi Learning.
3. Kalsi, P.S. (2004). *Spectroscopy of Organic Compounds*, New Age International Ltd.
4. Kemp, W. (1991). *Organic spectroscopy*, ELBS London.

5. Khopkar, S.M. (2007). *Basic Concepts of Analytical Chemistry*, New Age International Pvt Ltd.
6. Melinda J.D., (2010). *Introduction to solid NMR Spectroscopy*, Wiley India Pvt Ltd
7. Mendham, J.; Denney, R.C.; Barnes, J. D.; Thomas, M. J. K. (2003). *Vogel's Textbook of Quantitative Chemical Analysis*, Pearson Education Pvt. Ltd., New Delhi.
8. Pavia, D.L.; Lampman, G. M. (2010). *Introduction to Spectroscopy*, G. S. Kriz, Harcourt College, NY.
9. Popov, A.I.; Halenga, K. (1991). *Modern NMR techniques and their Applications*, Marcel Dekker.
10. Silverstein, R.M. (2006). *Spectrometric Identifications of Organic Compounds*, John Wiley.
11. Skoog, D.A.; West, D.M.; Holler, F.J.; Crouch, S.R. (2004). *Fundamental of Analytical Chemistry*, Saunders College Publishing, New York.
12. Willard, H.H.; Merrit, L.L.; Dean, J.A.; Settle, F.A. (2001). *Instrumental methods of analysis*, CBS Publishers and Distributors.
13. Williams, D.H.; Fleming, I. (2004). *Spectroscopy Methods in Organic Chemistry*, Tata McGraw-Hill Publishing Co. Ltd., New Delhi.

**Course Title: Organic Chemistry-Practical**

**Paper Code: CHM.506**

**Total Lectures: 36**

L	T	P	Credits	Marks
-		4	2	50

**A. Techniques:** (At least One Practical of Each Technique)

Crystallization, Fractional Crystallization, Sublimation, Distillation, Fractional Distillation, Steam Distillation, Vacuum Distillation, Column Chromatography, Thin Layer Chromatography (Purity would be checked by m. p. and mixed m. p.).

**B. Preparation of Derivatives:** (Each Derivative of two Compounds) Oxime, 2, 4-DNP, Acetyl, Benzoyl, Semicarbazone, Anilide, Amide, Aryloxyacetic acid.

**C. Preparations: Single Stage (Any 15)**

- 1 Cyclohexanone to Adipic acid
- 2 Benzophenone to Benzhydral
- 3 Chlorobenzene to 2,4-Dinitrochlorobenzene
- 4 2,4-Dinitrochlorobenzene to 2,4-Dinitrophenol
- 5 Acetoacetic ester to 1-Phenyl-3-methyl-5 pyrazolone
- 6 Benzaldehyde to Cinnamic acid
- 7 4-Chlorobenzaldehyde to 4-Chlorobenzoic acid + 4-Chlorobenzyl alcohol
- 8 Benzene to  $\beta$ -Benzoyl propionic acid
- 9 Benzaldehyde to Dibenzylidene acetone
- 10 p-Aminobenzoic acid to p-Chlorobenzoic acid
- 11 N,N-Dimethylaniline to 4-Formyl-N, N-dimethyl aniline
- 12 Benzophenone to Benzpinacol
- 13 p-Nitrotoluene to p-Nitrobenzoic acid
- 14 Anisole to 2,4-Dinitroanisole
- 15 Phthalic anhydride to phthalimide
- 16 Phthalimide to Anthranilic acid
- 17 Acetanilide to p-Bromoacetanide
- 18 p-Bromoacetanide to p-Bromoaniline
- 19 m-Dinitrobenzene to m-Nitroaniline
- 20 Synthesis of Phenytoin

**D. Use of Computer - Chem Draw-Sketch, ISI – Draw:** Draw the structure of simple aliphatic, aromatic, heterocyclic organic compounds with substituents. Get the correct IUPAC name and predict the UV, IR and  $^1\text{H-NMR}$  signals.

- E. Demonstration of Stereochemical aspects of the compounds through molecular models.

**ESSENTIAL BOOKS:**

1. Harwood, L.M., Moody, C.J. *Experimental Organic Chemistry*, 1st edition, Blackwell Scientific Publishers, 1989.
2. Vogel, A.I. *Text Book of Practical Organic Chemistry*, ELBS, IVth edition, Longman Group Ltd., 1978.
3. Mann, F.G.; Saunders, B.C. *Practical Organic Chemistry*, 4th edition, New Impression, Orient Longman Pvt. Ltd., 1975.
4. Leonard, J.; Lygo, B. *Advanced Practical Organic Chemistry*, Chapman and Hall, 1995.
5. Armarego, W. L., & Chai, C. (2012). *Purification of laboratory chemicals*. Butterworth-Heinemann.
6. Young, J. A. (Ed.). (Latest Edition). *Improving safety in the chemical laboratory: a practical guide*. Wiley.

**Course Title: Inorganic Chemistry Practical**  
**Paper Code: CHM.507**  
**Total Lectures: 36**

L	T	P	Credits	Marks
-		4	2	50

### **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.
3. Determination of ammonium / potassium thiocyanate.

### **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.

### **ESSENTIAL BOOKS:**

1. Pass, G.; Sutcliffe *Practical Inorganic Chemistry*, 1st edition, Chapman and Hall Ltd., 1968.
2. Jolly, W.L. *Synthetic Inorganic Chemistry*, 2nd edition, Prentice Hall, Inc., 1961.
3. Nakamoto, Kazuo *Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A and B*, 5th edition, John Wiley and Sons, 1997.
4. Mendham, J; Denney, R.C.; Barnes, J.D.; Thomas, M. *Vogel's Textbook of Quantitative Chemical Analysis*, 6th edition, Pearson Education, Ltd., 2000.
5. Svehla, G. and Sivasankar, B. *Vogel's Qualitative Inorganic Analysis (revised)*, Pearson, 7<sup>th</sup> edition, 1996.

## Interdisciplinary courses offered for Students of other Centres

Course Title: Chemistry without Test Tube (ID)

L	T	P	Credits	Marks
2	1	0	2	50

Total Hours: 36

### Unit 1 9 Hours

**How Science Deals with Complex problems:** Level in science, what are molecules made of, interaction between atoms, simplest examples: H<sub>2</sub> and LiH. Thinking in 3D, must we use quantum theory.

### Unit 2 9 Hours

**Electronic Structure:** What we know about atoms and molecules; atomic electronic structure, empirical chemistry; what is an orbital (atomic and molecular). Strategy for electronic structure, the Pauli principle and orbitals. Polyatomic Molecules: Methane, electronic structure of methane, shape of the methane molecule, chemist's description of methane.

### Unit 3 9 Hours

**Lone pairs of electrons:** Why are Not all electrons involved in bonding? What is a lone pair? Shapes of the simple molecules.

**Organic molecules with multiple bonds:** Double and triple bonds, ethene and methanal, reactivity of a double bond.

**Diatomics with multiple bonds:** N<sub>2</sub>, CO, O<sub>2</sub>

**Dative Bonds:** Solvation, reactive lone pair

Delocalized electronic substructures: The benzene molecule, delocalized electrons.

### Unit 4 9 Hours

**Reactions:** What makes a reaction to go? Formation of H<sub>2</sub> from H<sup>+</sup> and H<sup>-</sup>. Formation of lithium borohydride. Nucleophilic, elimination and addition reactions.

#### ESSENTIAL BOOKS:

1. Physical Chemistry: A Molecular Approach, D. A. McQuarrie, and J. D. Simon, Viva Books, 2011.
2. A. R. Leach, Molecular Modelling Principles and Applications, Prentice Hall (2001).
3. Introduction to Computational Chemistry, F. Jensen, 2<sup>nd</sup> edition, Wiley-Blackwell (2006).
4. Quantum Chemistry: A Unified Approach, D. B. Cook, 2<sup>nd</sup> edition, Imperial College Press (2012).
5. Why Chemical Reactions Happen, J. Keeler, P. Wothers, Oxford University Press (2003).
6. Reaction Dynamics, M. Brouard, Oxford Chemistry Primers (1998).

**Course Title: Spectroscopy in Drug Development and Analyses**

L	T	P	Credits	Marks
2		0	2	50

**Total Lectures: 36****Unit 1****9 Hours**

**UV-Visible spectroscopy:** Principle of UV-Visible Spectroscopy, Chromophores and their interaction with UV-visible radiation and their utilization in structural, qualitative and quantitative analysis of drug molecules. Woodward-Fieser rule, solvent effects

**Unit 2****9 Hours**

**Infrared spectroscopy:** Infrared radiation and its interaction with organic molecules, Determination of functional groups of drug molecules by IR, interpretation of IR spectra, FTIR.

**Unit 3****9 Hours**

**Nuclear magnetic resonance spectroscopy:** Applications of NMR for determining the structure of drug molecules, <sup>1</sup>H- NMR spectra, <sup>13</sup>C NMR, DEPT, HMQC, HMBC, quantitative analysis

**Unit 4****9 Hours**

**Mass spectrometry:** Basic principles and brief outline of instrumentation, Applications of mass spectroscopy for determining the structure of the drug, GC, LC

**Suggested Readings:**

1. Banwell, C.N.; McCash, E. M. (2000). *Fundamentals of molecular spectroscopy*, Tata McGraw-Hill, 4<sup>th</sup> edition, New Delhi.
2. Dyer, J.R. (2009). *Application of Absorption Spectroscopy of Organic Compounds*, PHI Learning, 2<sup>nd</sup> edition.
3. Kalsi, P.S. (2004). *Spectroscopy of Organic Compounds*, New Age International Ltd., 6<sup>th</sup> edition, New Delhi.
4. Kemp, W. (1991). *Organic spectroscopy*, ELBS London, 2<sup>nd</sup> edition.
5. Khopkar, S.M. (2007). *Basic Concepts of Analytical Chemistry*, New Age International Pvt Ltd.
6. Melinda J.D., (2010). *Introduction to solid-state NMR Spectroscopy*, Blackwell publishing, Oxford UK.
7. Mendham, J.; Denney, R.C.; Barnes, J. D.; Thomas, M. J. K. (2003). *Vogel's Textbook of Quantitative Chemical Analysis*, Pearson Education Pvt. Ltd., 6<sup>th</sup> edition, New Delhi.
8. Pavia, D.L.; Lampman, G. M. (2010). *Introduction to Spectroscopy*, G. S. Kriz, Harcourt College, 4<sup>th</sup> edition, NY.
9. Popov, A.I.; Halenga, K. (1991). *Modern NMR techniques and their Applications in Chemistry*, Marcel Dekker.
10. Sethi, P. D.; Sethi, R. (2007). *HPLC: High performance of liquid chromatography*, Vol 2, CBS Publishers and Distributors.

11. Silverstein, R.M. (2006). *Spectrometric Identifications of Organic Compounds*, John Wiley, 6<sup>th</sup> edition, .
12. Skoog, D.A.; West, D.M.; Holler, F.J.; Crouch, S.R. (2004). *Fundamental of Analytical Chemistry*, Saunders College Publishing, 7<sup>th</sup> edition, New York.
13. Willard, H.H.; Merrit, L.L.; Dean, J.A.; Settle, F.A. (2001). *Instrumental methods of analysis*, CBS Publishers and Distributors, 2<sup>nd</sup> edition.
14. Williams, D.H.; Fleming, I. (2004). *Spectroscopy Methods in Organic Chemistry*, Tata McGraw-Hill Publishing Co. Ltd., 7<sup>th</sup> edition, New Delhi.

**Course Title: Chemicals of Everyday life**

L	T	P	Credits	Marks
2	0	0	2	50

**Total Lectures: 36**

**Unit 1** **9Hours**

**Chemicals and safety**

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

**Unit 2** **9Hours**

**Common chemical processes**

Chemical reactions, Basics of organic synthesis, Chemistry of photosynthesis, Rusting, Electrochemical cells, Metal electroplating, Acid base titration in the lab

Use of polymers in daily life, Polymer based products, Teflon, Polystyrene, Plastic bags, ATM cards.

**Unit 3** **9 Hours**

**Chemistry of small bioactive molecules**

Caffeine, Nicotine, Paracetamol, Aspirin, DNA and RNA bases, Carbohydrates

Abused substances like morphine, Cannabis, Cocaine etc.

**Unit 4** **9 Hours**

**Green chemical processes**

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

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

**Suggested Readings**

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

**Course Title: Diseases and Medicines**  
**Paper Code: XXX**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Credits</b>	<b>Marks</b>
2	0	0	2	50

**Unit 1**

**18 Hours**

General awareness of Life style diseases like hypertension, diabetes, etc. management, use of medicines, and their side effects. General awareness of cancer and medicines for their treatment and management along with their side effects.

**Unit 2**

**18 Hours**

General awareness of Viral, bacterial, or other infectious diseases, precautions, medicines, their uses and side effects. General awareness of cancer and medicines for their treatment and management along with their side effects.

***Suggested Readings:***

1. Brunton, Laurence L., John S. Lazo, and Keith L. Parker. "Goodman and Gilman's the pharmacological basis of therapeutics." *McGraw-Hill, New York, Latest Edition.*
2. Tripathi, K. D. *Essentials of medical pharmacology.* JP Medical Ltd, 2013.  
Katzung, Bertram G., ed. "Basic & clinical pharmacology." *Latest Edition.*

## SEMESTER 2

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	Weightage				E
								A	B	C	D	
1	CHM.508	Inorganic Chemistry-II	CC	4	1	0	4	25	25	25	25	100
2	CHM.509	Organic Chemistry-II	CC	4	1	-	4	25	25	25	25	100
3	CHM.510	Physical Chemistry-II	CC	4	1	-	4	25	25	25	25	100
4	CHM.511	Quantum Chemistry-I	EC	4	1	-	4	25	25	25	25	100
5	CHM.512	Physical Chemistry - Practical	CC	-	-	4	2	-	-	-	-	50
6	CHM.513	Inorganic Chemistry-Practical	CC	-	-	4	2	-	-	-	-	50
7	CHM.514	Seminar in Chemical Sciences	FC	-	-	-	2	-	-	-	-	50
8	XXX	ID	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:** Continuous Assessment: Subjective by enlarge

**B:** Mid-Term Test-1: Based on Objective Type & Subjective Type Test

**C:** Mid-Term Test-2: Based on Objective Type & Subjective Type Test

**D:** End-Term Exam (Final): Based on Objective Type Tests

**E:** Total Marks

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

**Course Title: Inorganic Chemistry-II**  
**Paper Code: CHM.508**  
**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Unit 1** **22 Hours**

**Reaction Mechanisms of Transition Metal Complexes**

Introduction, ligand replacement reactions, classification of mechanisms, Water exchange rates, formation of complexes from aqueous ions, catanation, reaction, aquation and base hydrolysis attack on ligands, reactions, of square planar complexes, mechanism of ligand displacement reactions; metal carbonyl reactions, reactions of binuclear carbonyls, associative reactions, species with 17 electron, electron transfer processes outer and inner sphere. The 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, stereochemical non-rigidity, stereochemically non-rigid coordination compounds, Trigonal bipyramidal molecules, systems with coordination number six or more, isomerization and recombination's, tris chelate complexes, metal carbonyl scrambling cluster, rotation within Co shells.

**Unit 2** **15 Hours**

Higher boranes, carboranes, metalloboranes and metallocarboranes, metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

**Unit 3** **15 Hours**

**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.

**Unit 4** **20 Hours**

**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.

**ESSENTIAL BOOKS:**

1. Cotton, F.A.; Wilkinson *Advanced Inorganic Chemistry*, 6th edition, John Wiley & Sons, 1999.
2. Huheey, James E. *Inorganic Chemistry: Principles of Structure and Reactivity*, 4<sup>th</sup> edition, Harper Collins College Publishers, 1993.
3. Greenwood, N.N. and Earnshaw, A. *Chemistry of the Elements*, 2nd edition, Butterworth-Heinemann, A division of Read Educational & Professional Publishing Ltd., 2001.

4. Lever, A.B.P. *Inorganic Electronic Spectroscopy*, 2nd edition, Elsevier Science Publishers B.V., 1984.
5. Carlin, Richard L. and Duyneveldt, A.J. Van *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*, 1st edition, Oxford university Press, 2006.
7. Earnshaw, A. *Introduction to Magnetochemistry*, Academic Press, 1968
8. Dutta, R.L.; Syanal, A. *Elements of Magneto chemistry*, 2nd edition, Affiliated East West Press, 1993.
9. Drago, Russell S. *Physical Methods for Chemists*, 2nd edition, Saunders College Publishing, 1992.

**Course Title: Organic Chemistry-II**

**Paper Code: CHM.509**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

### Unit 1

**14 hours**

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

**Aromaticity:** Benzenoid and non-benzenoid compounds – generation and reactions.

### Unit 2

**20 hours**

**Synthetic methodologies:** Synthon, Synthetic equivalent, Functional group interconversion (FGI), Functional group addition, Functional group elimination, Criteria for selection of target, Linear and convergent synthesis, Retrosynthetic analysis and synthesis involving chemoselectivity, Regioselectivity, Reversal of Polarity (Umpolung), Synthesis of cyclic molecules, Strategic bond: Criteria for disconnection of strategic bonds, 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, One group C-C disconnections, alcohol and carbonyl compounds, regioselectivity, alkene synthesis, 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

**16 hours**

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

**Selective Name Reactions:** Aldol, Perkin, Stobbe, Dieckmann Condensation, Reimer-Tiemann, Reformatsky Grignard reactions, Diels-Alder reaction, Robinson Annelation, Michael addition, Mannich reaction, Stork-enamine, Sharpless Asymmetric Epoxidation, Ene, Barton, Hofmann-Löffler Fretag, Shapiro reaction, Chichibabin Reaction.

### Unit 4

**22 hours**

#### **Pericyclic chemistry:**

Introduction, Main features of pericyclic reactions, Classification of pericyclic reactions. 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. Thermal and photochemical pericyclic reactions.

Electrocyclic reactions: Conrotation and disrotation, Electrocyclic closure and opening in  $4n$  and  $4n+2$  systems. Woodward-Hoffmann selection rules for electrocyclic reactions. Explanation for the mechanism of electrocyclic reactions by (i) symmetry properties of

HOMO of open chain partner (ii) Conservation of orbital symmetry and orbital symmetry correlation diagrams and (iii) Huckel-Mobius aromatic and antiaromatic transition state method. Examples of electrocyclic reactions.

Cycloaddition reactions: Suprafacial and antarafacial interactions.  $\pi^2 + \pi^2$  and  $\pi^4 + \pi^2$  cycloadditions. Cycloreversions. Stereochemical aspects in supra-supra, supra-antara, antarsupra and antara-antara  $\pi^2 + \pi^2$  and  $\pi^4 + \pi^2$  cycloadditions. Diels-Alder reaction. Woodward-Hoffmann Selection rules for cycloaddition reactions. Explanation for the mechanism of cycloaddition reactions by (i) Conservation of orbital symmetry and orbital symmetry correlation diagrams (ii) Fukui Frontier Molecular Orbital (FMO) theory and (iii) Huckel-Mobius aromatic and antiaromatic transition state method. Endo-exo selectivity in Diels-Alder reaction and its explanation by FMO theory. Examples of cyclo addition reactions.

Sigmatropic reactions: [1,j] and [i,j] shifts; Suprafacial and antarafacial shifts; Selection rules for [l] shifts; Cope and Claisen rearrangements; Explanation for the mechanism of sigmatropic reactions 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.

### ***Suggested Readings:***

1. Acheson, R.M. (1976). *An introduction to the Chemistry of heterocyclic compounds*, Wiley India Pvt. Ltd., 3<sup>rd</sup> edition.
2. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2012). *Organic chemistry Organic Chemistry* Oxford press, 2<sup>nd</sup> edition
3. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., 4<sup>th</sup> edition, India.
4. Bansal, R. K., (2012). *Organic Reaction Mechanism*, New Age International (P) Ltd., 4<sup>th</sup> edition, New Delhi.
5. Bansal, R. K., (2007). *A text book of Organic Chemistry*, New Age International (P) Ltd., 5<sup>th</sup> edition, New Delhi.
6. Bansal, R.K. (2010). *Heterocyclic Chemistry*, New Age International (P) Ltd., 5<sup>th</sup> edition, New Delhi.
7. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B*, Springer, 5<sup>th</sup> edition.
8. Finar, I. L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, 6<sup>th</sup> edition, UK.
9. Gilchrist, T.L. (1997). *Heterocyclic Chemistry*, Longman, Prentice Hall, 3<sup>rd</sup> edition, US.
10. Gupta R.R., Kumar M., Gupta V. (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3*, Springer Verlag, India.
11. Joule, J.A., Mills, K. (2010). *Heterocyclic Chemistry*, Blackwell Publishers, 5<sup>th</sup> edition, New York.
12. Kalsi P. S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Publication, 3<sup>rd</sup> edition, New Delhi.

13. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3<sup>rd</sup> edition, US.
14. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
15. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
16. R. Katritzky, (2010). *Handbook of Heterocyclic Chemistry* Elsevier, 3<sup>rd</sup> edition, UK.
17. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
18. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, US.
19. Norman, R.O.C.; Coxon, J.M. *Principles of Organic Synthesis*, Blackie Academic & Professional.
20. Warren, S., (2010). *Organic synthesis: The Synthron Approach*. John wiley & Sons, New York,
21. Warren, S., (2010). *Designing organic synthesis: A Disconnection Approach*. John Wiley & Sons, New York.
22. Corey E.J., Cheng Xue-Min, *The Logic of Chemical Synthesis*, Pubs: John Wiley & Sons, (1989).

**Course Title: Physical Chemistry-II**

**Paper Code: CHM.510**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Unit 1** **20 Hours**

**Properties of Gases:** Ideal gases, two-parameter equations of state, cubic equation of state for gaseous and liquid states, van der Waals constants in terms of molecular parameters.

**Statistical Thermodynamics:** The canonical ensemble, distribution law, partition functions for ideal gas: translational, rotational, vibrational, electronic partition functions. Calculation of Thermodynamic properties in terms of partition functions, Heat capacity, behavior of solids chemical equilibria and equilibrium constant in terms of partition function.

**Unit 2** **16 Hours**

**Thermodynamics:** The First Law of Thermodynamics, Entropy and the Second Law, Entropy and the Third Law of Thermodynamics. Helmholtz and Gibbs Energies, Phase Equilibria.

**Unit 3** **18 Hours**

**Chemical Equilibrium:** Gibbs energy is a minimum with respect to the extent of reaction, Equilibrium constant as a function of temperature, Standard Gibbs energies and Equilibrium constant, Direction of reaction spontaneity, Van't Hoff equation, Molecular partition functions and related thermodynamic data.

**Unit 4** **18 Hours**

**Liquid-Liquid Solutions:** Partial molar quantities, Gibbs-Duhem equation, Raoult's and Henry's law.

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

**ESSENTIAL BOOKS:**

1. Physical Chemistry, G. M. Barrow, TATA MCGRAW-HILL, 2007.
2. Text Book of Physical Chemistry, K. L. Kapoor, MACMILLAN, 2006.
3. Physical Chemistry, A. W. Atkins, W. H. Freeman, and Company, 1997.
4. Physical Chemistry: A Molecular Approach, D. A. McQuarrie, and J. D. Simon, Viva Books, 2011.
5. Kinetics and Mechanism, J. W. Moore, and R. G. Pearson, John Wiley and Sons, 1981.
6. Physical Chemistry, R. J. Silbey, R. A. Alberty, and M. G. Bawendi, Wiley-Interscience Publication, 2013.
7. Physical Chemistry, T. Engel, and P. Reid, Prentice-Hall, 2012.

**Course Title: Quantum Chemistry-I**

**Paper Code: CHM.511**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Unit 1** **20 Hours**

**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 tunneling effect, one-dimensional harmonic oscillator and rigid rotor. Angular momentum, eigenvalues of angular momentum operator, Particle in a Ring, Hydrogen Atom.

**Unit 2** **14 Hours**

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

**Unit 3** **18 Hours**

**Symmetry Point Groups:** Determination of point group of a molecule, representations, the great orthogonality theorem, character table, and construction of character tables for  $c_{2v}$  and  $c_{3v}$  groups, symmetry adapted atomic basis sets, construction of molecular orbitals. The direct product representation.

**Unit 4** **20 Hours**

**Atomic and Molecular Structure:** many electron wave functions, Pauli Exclusion Principle, Helium atom, atomic term symbols. The self-consistent field method. Slater-type orbitals. Born-Oppenheimer approximation. Molecular orbital treatment for  $H_2^+$ . MO treatment of homo- and hetero nuclear diatomic molecules. Hückel mo treatment of simple and conjugated polyenes and alternate hydrocarbons.

**Recommended books:**

1. Quantum Chemistry, I.N. Levine, 5<sup>th</sup> edition, Pearson Educ., Inc. New Delhi (2000).
2. Physical Chemistry: A Molecular Approach, D. A. McQuarrie, and J. D. Simon, Viva Books (2011).
3. Valence Theory, J.N. Murrell, S.F.A. Kettle and J. M. Tedder, 2<sup>nd</sup> edition, John Wiley (1965).
4. Introductory Quantum Chemistry, A.K. Chandra, 4<sup>th</sup> Edition, Tata Mcgraw Hill (1994).
5. Chemical Applications of Group Theory, F. A. Cotton, John Wiley & Sons (2008).
6. Molecular Symmetry and Group Theory, R. L. Carter, J. Wiley (1998).
7. Group Theory and Chemistry, D. M. Bishop, Dover Publications (1993).
8. Quantum Chemistry, J. P. Lowe, and Peterson, K., Academic Press (2005).

**Course Title: Physical Chemistry-Practical**  
**Paper Code: CHM.512**  
**Total Lectures: 36**

L	T	P	Credits	Marks
		4	2	50

1. Comparison of acid strengths through acid catalyzed methyl acetate hydrolysis.
2. Energy of activation of acid catalyzed hydrolysis of methyl acetate.
3. Determination of partition coefficient of iodine between water and CCl<sub>4</sub>/equilibrium constant of tri-iodide formation.
4. Conductometric titration of a weak acid with strong base.
5. Conductometric titration of a mixture of weak and strong acids.
6. Potentiometric titration of a strong acid with strong base using quinhydrone electrode.
7. Conductometric titration of KCl with AgNO<sub>3</sub>.
8. Molecular weight of a non-electrolyte by cryoscopy method.
9. Plateau of GM tube and study of counting statistics.
10. Determination of half-life of a radionuclide.
11. To determine the amount of acetic acid adsorbed at its different concentrations by charcoal and hence verify the Freundlich adsorption isotherm.
12. Determination of dimerisation constant of benzoic acid in benzene solution.

**ESSENTIAL BOOKS:**

7. An advanced course in practical chemistry, A. K. Nad, B. Mahapatra, and A. Ghoshal, New Central Book Agency (P) Ltd (2000).
8. Physical Chemistry Practical, S. Maity and N. Ghosh, New Central Book Agency (P) Ltd (2012).
9. Collection of Interesting General Chemistry Experiments, A. J. Elias, Universities Press (2008).

**Course Title: Inorganic Chemistry Practical****Paper Code: CHM.513****Total Lectures: 36**

L	T	P	Credits	Marks
		4	2	50

1. Preparation of Chloropentaammine cobalt (III) Chloride and its IR measurements.
2. Preparation of  $[\text{Co}(\text{en})_2\text{Cl}_2]\text{Cl}$ ,  $\text{Na}_2[\text{Fe}(\text{CN})_5\text{NH}_3] \cdot \text{H}_2\text{O}$ ,  $[\text{UO}_2(\text{NO}_3)_2 \cdot 2\text{Py}]$ ,  $\text{Cu}_2(\text{CH}_3\text{COO})_4(\text{H}_2\text{O})_2$ .
3. Preparation of  $\text{Hg}[\text{Co}(\text{CNS})_4]$  and to study its properties.
4. Preparation of cis-and trans- $\text{K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$  and its IR study.
5. Preparation of bis(2,4-pentanedione)vanadium(IV) acetate and its piperidine or pyridine complex.
6. Study of both the complexes with the help of infrared, UV-vis spectroscopy and magnetic susceptibility.
7. Preparation of lead tetraacetate.

**ESSENTIAL BOOKS:**

1. Pass, G.; Sutcliffe *Practical Inorganic Chemistry*, 1st edition, Chapman and Hall Ltd., 1968.
2. Jolly, W.L. *Synthetic Inorganic Chemistry*, 2nd edition, Prentice Hall, Inc., 1961.
3. Kolthoff, I.M.; Sanddl, E.B. *Text Book of Quantitative Inorganic Analysis*, Revised Edition, London Macmillan and Co. Ltd., 1950.
4. Nakamoto, Kazuo *Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A and B*, 5th edition, John Wiley and Sons, 1997.
5. Mendham, J; Denney, R.C.; Barnes, J.D.; Thomas, M. *Vogel's Textbook of Quantitative Chemical Analysis*, 6th edition, Pearson Education, Ltd., 2000.
6. Marr, G. and Rockett, B.W. *Practical Inorganic Chemistry*, Van Nostrand Reinhold Company. 7. Jolly, W.L. *The Synthesis and Characterization of Inorganic Compounds*. Prentice Hall.

### SEMESTER 3

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	Weightage				E
								A	B	C	D	
1	CHM.601	Inorganic Chemistry-III	CC	4	1	-	4	25	25	25	25	100
2	CHM.602	Organic Chemistry-III	CC	4	1	-	4	25	25	25	25	100
3	CHM.603	Physical Chemistry-III	CC	4	1	-	4	25	25	25	25	100
4	CHM.604	Research Methodologies	FC	2	-	-	2	10	15	15	10	50
5	CHM.605	Biostatistics	FC	2	-	-	2	10	15	15	10	50
6	CHM.606	Practical Inorganic Chemistry	EC	-	-	4	2	-	-	-	-	50
	CHM.607	Practical Organic Chemistry										
	CHM.608	Practical Physical Chemistry										
7	CHN.609	Seminar	FC	-	-	-	2	-	-	-	-	50
<b>Opt any one course from following elective courses</b>												
8	CHM.610	Current trends in Organic synthesis	EC	4	1	-	4	25	25	25	25	100
	CHM.611	Introduction to Medicinal Chemistry										
	CHM.612	Nuclear Chemistry										
	CHM.613	Inorganic Photochemistry										
	CHM.614	Quantum Chemistry-II										
	CHM.615	Material Chemistry										
<b>Total</b>				<b>20</b>	<b>4</b>	<b>4</b>	<b>24</b>					<b>600</b>

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

**A:** Continuous Assessment: Subjective by enlarge

**B:** Mid-Term Test-1: Based on Objective Type & Subjective Type Test

**C:** Mid-Term Test-2: Based on Objective Type & Subjective Type Test

**D:** End-Term Exam (Final): Based on Objective Type Tests

**E:** Total Marks

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

**Course Title: Inorganic Chemistry-III**

**Paper Code: CHM.601**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Unit 1**

**28 Hours**

**Lanthanides, actinides and super-heavy elements**

Coordination chemistry, magnetic and spectral properties, comparison of general properties of lanthanides and actinides, comparison with d-block elements, 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.

**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.

**Unit 2**

**20 Hours**

**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  $[\text{BH}_3]$ -

**Unit 3**

**12 Hours**

**Mossbauer Spectroscopy**

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

**Unit 4**

**12 Hours**

**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.

**ESSENTIAL BOOKS:**

1. Drago, Russell S. *Physical Methods for Chemists*, 2nd edition, Saunders College Publishing, 1992.
2. Ebsworth, E.A.V.; Rankin, D.W.H.; Craddock, S. *Structural Methods in Inorganic Chemistry*, 1st edition, ELBS, 1987.

3. Cotton, F.A.; Lippard, S.J. *Progress in Inorganic Chemistry*, Vol. 8, Vol. 15, Wiley Internationals.
4. Lever, A.B.P. *Inorganic Electronic Spectroscopy*, 2nd edition, Elsevier Science Publishers B.V., 1984.
5. Parish, R.V. *NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry*, 1st edition, Ellis Harwood, 1990.
6. Silverstein, R.M.; Bassler, G.C.; Morrill, T.C. *Spectrometric Identification of Organic Compounds*, 6th edition, John Wiley, 2002.
7. Abraham, R.J.; Fisher, J.; Loftus, P. *Introduction to NMR Spectroscopy*, Wiley.
8. Dyer, J.R. *Application of Spectroscopy of Organic Compounds*, Prentice Hall.
9. Nakamoto, Kazuo *Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A and B*, 5th edition, John Wiley and Sons, 1997
10. Carlin, R.I. *Transition Metal Chemistry*, Vol. 3, Dekker
11. Martin, M.L.; Delpeuch, J.J.; Martin, G.J. *Practical NMR Spectroscopy*, Heyden
12. Williams, D.H.; Fleming, I. *Spectroscopic Methods in Organic Chemistry*, Tata McGraw-Hill.
13. Greenwood, Norman Neill, and Alan Earnshaw. "Chemistry of the Elements." (1984).
14. Ozin, Geoffrey A., André C. Arsenault, and Ludovico Cademartiri. *Nanochemistry: a chemical approach to nanomaterials*. Royal Society of Chemistry, 2009.
15. Klabunde, Kenneth J., and Ryan M. Richards, eds. *Nanoscale materials in chemistry*. John Wiley & Sons, 2009.

**Course Title: Organic Chemistry-III****Paper Code: CHM.602****Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Unit 1****16 hours**

**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****16 hours**

**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****18 hours**

**Metal and non-metal mediated oxidation and reductions:** Mechanism, Selectivity, Stereochemistry and applications of oxidation reactions, Oppenauer, Baeyer-Villiger, Oxidation reactions using DDQ, NBS, lead tetraacetate, selenium dioxide, DCC, PCC, CAN, Cr and Mn reagents, periodic acid, Osmium tetroxide, Swern oxidations, Hydroboration, Dehydrogenation, Ozonolysis, Epoxidations using peracids.

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 Rh catalysis, Boron in reduction.

**Unit 4****22 hours**

**Heterocyclic chemistry:** Replacement and 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

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

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

(c) Benzo-fused five-membered and six membered heterocycles: Synthesis and reactions of indoles, benzofurans and benzimidazoles, benzothiazoles, imidazopyridine, pyrrolopyridine/pyrimidines.

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

**Suggested Readings:**

1. Acheson, R.M. (1976). *An introduction to the Chemistry of heterocyclic compounds*, Wiley India Pvt. Ltd., 3<sup>rd</sup> edition.
2. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., 4<sup>th</sup> edition, India.
3. Bansal, R. K., (2012). *Organic Reaction Mechanism*, New Age International (P) Ltd., 4<sup>th</sup> edition, New Delhi.
4. Bansal, R. K., (2007). *A text book of Organic Chemistry*, New Age International (P) Ltd., 5<sup>th</sup> edition, New Delhi.
5. Bansal, R.K. (2010). *Heterocyclic Chemistry*, New Age International (P) Ltd., 5<sup>th</sup> edition, New Delhi.
6. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B*, Springer, 5<sup>th</sup> edition.
7. Finar, I. L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, 6<sup>th</sup> edition, UK.
8. Gilchrist, T.L. (1997). *Heterocyclic Chemistry*, Longman, Prentice Hall, 3<sup>rd</sup> edition, US.
9. Gupta R.R., Kumar M., Gupta V. (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3*, Springer Verlag, India.
10. Joule, J.A., Mills, K. (2010). *Heterocyclic Chemistry*, Blackwell Publishers, 5<sup>th</sup> edition, New York.
11. Kalsi, P. S., (2008). *Stereochemistry: Conformation and Mechanism*, New Age International (P) Ltd., 7<sup>th</sup> edition, India.
12. Kalsi P. S., (2014). *Organic Reactions and Their Mechanisms*, New Age International Publication, 3<sup>rd</sup> edition, New Delhi.
13. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3<sup>rd</sup> edition, US.
14. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
15. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
16. R. Katritzky, (2010). *Handbook of Heterocyclic Chemistry* Elsevier, 3<sup>rd</sup> edition, UK.
17. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
18. Joule, J.A., Mills, K. (2010). *Heterocyclic Chemistry*, Blackwell Publishers, 5<sup>th</sup> edition, New York.
19. Kalsi, P. S., (2008). *Stereochemistry: Conformation and Mechanism*, New Age International (P) Ltd., 7<sup>th</sup> edition, India.
20. Kalsi P. S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Publication, 3<sup>rd</sup> edition, New Delhi.
21. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3<sup>rd</sup> edition, US.

22. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
23. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
24. R. Katritzky, (2010). *Handbook of Heterocyclic Chemistry* Elsevier, 3<sup>rd</sup> edition, UK.
25. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.

**Course Title: Physical Chemistry-III**

**Paper Code: CHM.603**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

### Unit 1

**20 Hours**

**Basic Principles:** Interaction of electromagnetic radiation with matter, time-dependent perturbation theory, harmonic perturbation and transition probabilities, Einstein transition probabilities, selection rules, line-widths and line shapes, Fourier Transforms in spectroscopy. Introduction to Electronic spectra, Born-Oppenheimer approximation, Franck-Condon principle, change of shape on excitation, Jablonski diagram: fluorescence and phosphorescence.

### Unit 4

**20 Hours**

**Infra-red and Raman Spectra:** Harmonic and anharmonic oscillators, fundamental frequencies, overtones, Morse potential, hot bands, vibration-rotational spectra of HCl, P, Q, R branches, vibrational theories of polyatomic molecules, normal coordinates and their symmetry (CO<sub>2</sub>). Molecular polarizability-Raman Effect, pure rotational Raman spectra of linear molecules, vibrational Raman spectra-Raman activity of vibrational, rule of mutual exclusion. Microwave spectra: rigid and non-rigid rotator mode ls, rotational energies of diatomic molecules: moment of inertia and bond length, centrifugal distortion, effect of isotopic substitution.

### Unit 3

**14 Hours**

**Magnetic Resonance:** Basic Principles, Nuclear Shielding, Chemical Shift, Spin-spin Coupling: AX, AMX, AX<sub>2</sub>, AX<sub>3</sub>, AX<sub>n</sub>, Equivalent Nuclei, Mechanism, Dipolar Coupling.

### Unit 4

**18 Hours**

**Lasers and Laser Spectroscopy:** Principles of laser action, laser characteristics, pulsed lasers, laser cavity modes, Q-switching, mode locking, non-linear effects, harmonic generation, examples of lasers: He-Ne, Nd-YAG, dye lasers, femtosecond spectroscopy.

### ESSENTIAL BOOKS:

1. Modern Spectroscopy, J. M. Hollas, 4th edition, John Wiley & Sons, Ltd. (2004).
2. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw-Hill (1962).
3. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E.M. Mc Cash, 4th edition, Tata McGraw Hill, New Delhi (1994).
4. Principle of Fluorescence Spectroscopy, L. R. Lakowicz, 3<sup>rd</sup> Edition, Springer.
5. Introduction to Magnetic Resonance A. Carrington and A. D. Mc Lachlan, Chapman and Hall, London (1979).
6. Nuclear Magnetic Resonance Spectroscopy, R. K. Harris, Addison Wesley, Longman Ltd, London (1986).

**Course Title: Research Methodology**  
**Paper Code: CHM.604**  
**Total Lectures: 36**

L	T	P	Credits	Marks
2	0	0	2	50

### Unit 1

**10 Hours**

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

**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 Hours**

**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 Hours**

**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.

#### ESSENTIAL BOOKS:

1. Gupta, S. (2005). *Research methodology and statistical techniques*, Deep & Deep Publications (p) Ltd. New Delhi.
2. Kothari, C. R. (2008.) *Research methodology(s)*, New Age International (p) Limited. New Delhi
3. Best J. W., Khan J. V. (Latest Edition) *Research in Education*, Prentice Hall of India Pvt. Ltd.
4. *Safe science: promoting a culture of safety in academic chemical research*; National Academic Press, www.nap.edu.
5. Copyright Protection in India [website: <http://copyright.gov.in>].
6. World Trade Organization [website: [www.wto.org](http://www.wto.org)].
7. Wadedhra B.L. Law Relating to Patents, Trademarks, Copyright Design and Geographical Indications. Universal Law Publishing, New Delhi. Latest Edition.

**Course Title: Biostatistics**

**Paper Code: CHM.605**

**Total Lectures: 36**

L	T	P	Credits	Marks
2	0	0	2	50

**Unit 1**

**10 Hours**

**Overview of biostatistics:** Difference between parametric and non-parametric statistics, Univariate and multivariate analysis, Confidence interval, Errors, Levels of significance, Hypothesis testing.

**Descriptive statistics:** Measures of central tendency and dispersal, Histograms, Probability distributions (Binomial, Poisson and Normal), Sampling distribution, Kurtosis and Skewness.

**Unit 2**

**5 Hours**

**Experimental design and analysis:** Sampling techniques, Sampling theory, various steps in sampling, collection of data-types and methods.

**Unit 3**

**12 Hours**

**Comparing means of two or more groups:** Student's t-test, Paired t-test, Mann-Whitney U-test, Wilcoxon signed-rank, One-way and two-way analysis of variance (ANOVA), Critical difference (CD), Least Significant Difference (LSD), Kruskal-Wallis one-way ANOVA by ranks, Friedman two-way ANOVA by ranks,  $\chi^2$  test.

**Unit 4**

**9 Hours**

**Regression and correlation:** Standard errors of regression coefficients, Comparing two regression lines, Pearson Product-Moment Correlation Coefficient, Spearman Rank Correlation Coefficient, Power and sampling size in correlation and regression.

**ESSENTIAL BOOKS:**

1. Norman, G. and Streiner, D. (3<sup>rd</sup> edn) (2008). *Biostatistics: The Bare Essentials*. Decker Inc., Canada.
2. Sokal, R.R. and Rohlf, F.J. (1994). *Biometry: The Principles and Practices of Statistics in Biological Research*, W.H. Freeman and Company, New York.

**Course Title: Practical Inorganic Chemistry**  
**Paper Code: CHM.606**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Credits</b>	<b>Marks</b>
0	0	4	2	50

### **Inorganic Chemistry**

1. Colorimetric estimation of cations and anions.
2. Separation techniques
  - i. Ion exchange
  - ii. Solvent extraction
  - iii. Column and paper chromatography

### **ESSENTIAL BOOKS:**

1. Pass, G.; Sutcliffe *Practical Inorganic Chemistry*, 1st edition, Chapman and Hall Ltd., 1968.
2. Jolly, W.L. *Synthetic Inorganic Chemistry*, 2nd edition, Prentice Hall, Inc., 1961.
3. Mauritis Kolthoff's and Saddle Text Book of Quantitative Inorganic Analysis.
4. Vogel, A.I. *Text Book of Practical Organic Chemistry*, ELBS, 5th edition, Longman Group Ltd., 1989.

**Course Title: Practical Organic Chemistry**  
**Paper Code: CHM.607**

L	T	P	Credits	Marks
0	0	4	2	50

### Organic Chemistry

- Organic Lab.
  - Safety: Eye, Fire and Chemicals
  - Glassware
  - Non-glass equipment
  - Heating devices
  - Cleaning Glassware
- Regioselective reduction of  $\alpha$ ,  $\beta$  unsaturated carbonyl compound under microwave irradiation.
- To study decarboxylation of Ferulic acid under microwave irradiation.
- Synthesis of biphenyl alcohol through Grignard reaction.
- Synthesis of bioactive stilbenes through one pot two step modified Perkins reaction.
- To synthesize 4-nitrobenzaldehyde oxime from p-nitrobenzaldehyde.
- To synthesize isooxazoline from prior synthesized oxime.
- Reduction of p-chlorobenzaldehyde using sodium borohydride ( $\text{NaBH}_4$ ).
- To mesylate the furfuryl alcohol.
- To synthesize substituted benzodiazepine from Chalcone via reflux conditions
- To synthesize Chalcone from o-nitrobenzaldehyde and p-hydroxy acetophenone under acidic condition
- To synthesize acylidine analogues of Meldrum acid.
- Synthesis of imidazole based ionic liquids
- To determine corrected melting points of an unknown organic compound (calibration of thermometer).
- Adipic acid from cyclohexanol (oxidation).
- p- Iodonitrobenzene from p-nitroaniline.
- Preparation of benzyl alcohol and benzoic acid (Cannizzaro's reaction).
- Cinnamic acid from benzaldehyde (Knoevenagel reaction).
- Separation of mixtures of organic compounds by means of chemical methods.

### ESSENTIAL BOOKS:

- Harwood, L.M., Moody, C.J. *Experimental Organic Chemistry*, 1st edition, Blackwell Scientific Publishers, 1989.
- Vogel, A.I. *Text Book of Practical Organic Chemistry*, ELBS, IVth edition, Longman Group Ltd., 1978.
- Mann, F.G.; Saunders, B.C. *Practical Organic Chemistry*, 4th edition, New Impression, Orient Longman Pvt. Ltd., 1975.
- Tewari, K.S.; Vishnoi, N.K.; Mehrotra, S.N. *A Textbook of Organic Chemistry*, 2<sup>nd</sup> edition, Vikas Publishing House, 1976.
- Leonard, J.; Lygo, B. *Advanced Practical Organic Chemistry*, Chapman and Hall, 1995.

**Course Title: Practical Physical Chemistry**  
**Paper Code: CHM.608**

<b>L</b>	<b>T</b>	<b>P</b>	<b>Credits</b>	<b>Marks</b>
0	0	4	2	50

**Physical Chemistry**

1. Gaussian09, Z-matrix, Cartesian Coordinate,
2. Potential energy surface, Force fields,
3. concept of Basis set (STO-3G, 3-21G, 6-31G, 6-31G\*, 6-31G\*\*),
4. The Born-Oppenheimer approximation, local and global minima,
5. Hartree-Fock approximation,
6. Kohn-Sham Equation
7. Density Functional Theory.
8. Determination of CMC of CTAB and SDS using conductivity and colorimetric methods
9. Determine the molecular weight of a given macromolecule (PVP) by the viscosity method.
10. Synthesis and Structural characterization of nanoiron.
11. Synthesis and characterization of micellar templated synthesis of CdSe nanomaterial.
12. Sol-gel Synthesis of ZnO nanoparticle.
13. Ligand capping of gold nanoparticles.
14. Nanomaterial synthesis using spray pyrolysis.
15. Thermogravimetric analysis of metal carbonates and evaluation of thermodynamic parameters

**ESSENTIAL BOOKS:**

1. Gaussian 09 Manuals

Course Title: Current Trends in Organic Synthesis

Paper Code: CHM.610

Total Lectures: 72

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), 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, 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.

**ESSENTIAL BOOKS:**

1. Finar, I.L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, 6<sup>th</sup> edition, UK.
2. Finar, I.L., (2012). *Organic Chemistry Vol. 2: Stereochemistry and The Chemistry of Natural Products*, Pearson Education, 6<sup>th</sup> edition, UK.
3. Fleming (1999). *Pericyclic Reactions*, Oxford University Press, Oxford.
4. Fleming (2010). *Molecular Orbitals and Organic Chemical Reactions*, John Wiley & Sons.
5. Jie Jack Li, (2009). *Name Reactions: A collection of Detailed Reaction Mechanism*, Publisher: Springer-verlag

6. Kalsi, P.S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Pub., 3<sup>rd</sup> edition, New Delhi.
7. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd., New Delhi.
8. Lowry, T.H., Richardson K.S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc.
9. Mc Murry, J., *Organic Chemistry*, Asian Book Pvt Ltd, New Delhi
10. Morrison, R.T., Boyd, R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
11. Mukherjee, S.M., Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
12. Reinhard Bruckner, (2001). *Advanced organic chemistry: Reaction Mechanism*, Academic Press.
13. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
14. Solomn, C.W.G, Fryble, C.B. (2003). *Organic Chemistry*, John Wiley & Sons, Inc., 8<sup>th</sup> edition, New York.
15. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, 6<sup>th</sup> edition, US.
16. W. Carruthers, (2004). *Some Modern Methods of Organic Synthesis*, Cambridge Uni. Press, 4<sup>th</sup> edition, UK.

**Course Title: Introduction to Medicinal Chemistry**

**Paper Code: CHM.611**

**Total Hours: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Unit 1** **12 Hours**

**History of drug discovery:** Introduction, Drug discoveries, Recent trends in drug discovery.

**Unit 2** **20 Hours**

**Medicinal chemistry:** Definitions and objectives, Drug activity phases, Drug classification system.

**Measurement and expression of drug effects:** Introduction, In-vitro experiments, Ex-vivo experiments, In-vivo experiments.

**Unit 3** **20 Hours**

**Molecular drug targets:** Introduction, Enzymes as drug targets, Membrane transporters as drug targets, Voltage-gated ion channels as drug targets, Non-selective cation-channels as drug targets, Direct ligand gated ion channels, Receptors with intrinsic enzyme activity, Receptors coupled to various cytosolic proteins, G-Protein coupled receptors, Nuclear receptors.

**Unit 4** **20 Hours**

**Drug targets, target identification, validation and screening:** Introduction, Improving the resolution of disease etiology, Biopharmaceutical therapies, Drug target identification, Hit to lead, Clinical biomarkers

**Suggested Readings:**

1. Delgado, J. N. and Remers W A, Ed. (2010). *Wilson & Gisvold's Textbook of Organic and Pharmaceutical Chemistry*, J. Lippincott Co., 7<sup>th</sup> edition, Philadelphia.
2. Foye, W. C. (2008). *Principles of Medicinal Chemistry*, Publisher: Lea and Febiger, 6<sup>th</sup> edition, Philadelphia.
3. King, F. D. (2003). *Medicinal Chemistry Principles and Practice*, Royale Society of Chemistry, 2<sup>nd</sup> Edition, London.
4. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, 3<sup>rd</sup> edition, New York.
5. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*, Oxford University Press, 4<sup>th</sup> edition. UK.
6. Singh, H., Kapoor, V.K. (Latest Edition). *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.
7. Smith, H.J. (2006). *Introduction to the Principles of Drug Design and Action*, Taylor and Francis, 4<sup>th</sup> edition, UK.
8. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier), 3<sup>rd</sup> edition.
9. Wolff, M E, Ed., (2010). *Burger's Medicinal Chemistry and Drug Discovery*, John Wiley and Sons, New York.

**Course Title: Nuclear Chemistry**

**Paper Code: CHM.612**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

### **Unit 1**

**16 Hours**

#### **Nuclear Structure and Stability**

Binding energy, empirical mass equation, nuclear models, the liquid drop model, the shell model, the Fermi gas model & collective nuclear model, nuclear spin, parity & magnetic moments of odd mass numbers nuclei.

### **Unit 2**

**20 Hours**

#### **Nuclear reaction**

Introduction, Production of projectiles, nuclear cross section, nuclear dynamics, threshold energy of nuclear reaction, Coulomb scattering, potential barrier, potential well, formation of a compound nucleus, Nuclear reactions, direct Nuclear reactions, heavy ion induced nuclear reactions, photonuclear reactions.

#### **Nuclear fission**

Liquid drop model of fission, fission barrier and threshold, fission cross section, mass energy and charge distribution of fission products, symmetric and Assymmetric fission, decay chains and delayed neutrons.

### **Unit 3**

**20 Hours**

#### **Reactor Theory**

Nuclear fission as a source of energy, Nuclear chain reacting systems, critical size of a reaction, research reactors, graphite moderated, heterogeneous, enriched uranium reactors, light water moderated, heterogeneous, enriched uranium reactors, water boilers enriched aq. Homogeneous reactors, Thermonuclear reactors, gamma interactions, shielding and health protection. Reactors in India.

#### **Nuclear Resources in India**

Uranium and Thorium resources in India and their extractions, Heavy water manufacturing in India.

### **Unit 4**

**16 Hours**

#### **Elements of Radiation Chemistry**

Radiation Chemistry, Interaction of radiation with matter, Passage of neutrons through matter, Interaction of gamma radiation with matter, Units for measuring radiation absorption, Radiolysis of water, Free radicals in water radiolysis, Radiolysis of some aqueous solutions

#### **ESSENTIAL BOOKS:**

1. Friedlander, Kennedy and Miller, Nuclear and Radio Chemistry: John Wiley
2. B.G. Harvey, Nuclear Chemistry
3. Hassinsky: Translated by D.G. Tuck, Nuclear Chemistry and its application: Addison Wiley
4. B.G. Harvey, Introduction to Nuclear Physics and Chemistry
5. Maeclefort: Nuclear Chemistry: D.Van Nostrand

6. An N.Nesmeyannoy: Radiochemistry: Mir
7. Jacobs et al: Basic Principles of nuclear Science and Reactors, V.Nost & EWAP
8. N. Jay: Nuclear Power Today Tomorrow: ELBS
9. Kenneth: Nuclear Power Today, Tomorrow: ELBS
10. Essentials of Nuclear Chemistry, H.J. Arnikar, John Wiley
11. Nuclear and Radiation Chemistry: B.K. Sharma, Krishna Publication
12. An Introduction to Nuclear Physics: R. Babber. and Puri

**Course Title: Inorganic Photochemistry**

**Paper Code: CHM.613**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

#### **UNIT I**

**18 Hours**

**Basics of photochemistry:** Absorption, excitation, photochemical laws, quantum yield, lifetime of excited states, Flash photolysis, stopped flow techniques. Energy dissipation by radiative and non-radiative process, absorption spectra, Franck-Condon principles, photochemical stages- primary and secondary process;

#### **UNIT II**

**18 Hours**

**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 III**

**18 Hours**

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

#### **UNIT IV**

**18 Hours**

**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.

#### **SUGGESTED READINGS**

1. Lackowicz, J. R. Principle of Fluorescence Spectroscopy, 2006.
2. Endicott, J. F., A. W. Adamson, and P. D. Fleischauer. Concepts of Inorganic Photochemistry. Wiley (1975).
3. Rohatgi-Mukherjee, K. K. Fundamentals of photochemistry. New Age International, 1978.
4. Kryukov, A. I., and S. Ya Kuchmii. "Fundamentals of Photochemistry of Coordination Compounds." (1990).

**Course Title: Quantum Chemistry-II**

**Paper Code: CHM.614**

**Total Hours: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Unit 1** **18 Hours**

**Many Electron atoms:** Electron correlation, addition of angular momentum, Clebsch-Gordan series, total angular momentum and spin-orbit interaction.

**Unit 2** **18 Hours**

**Ab Initio Methods:** Review of molecular structure calculations, Hartree-Fock SCF method for molecules, Roothaan-Hartree-Fock method, and selection of basis sets.

**Unit 3** **18 Hours**

**Electron Correlation and Basis Sets:** Configuration Interaction, Multi-Configuration Self-Consistent Field, Multi-Reference Configuration Interaction, Many-Body Perturbation Theory, Coupled Cluster, Basis sets.

**Unit 4** **18 Hours**

**DFT and Force Fields method:** Energy as a functional of charge density, Kohn-Sham equations. Molecular mechanics methods, minimization methods, QSAR.

**ESSENTIAL BOOKS:**

1. Introduction to Computational Chemistry, F. Jensen, 2<sup>nd</sup> edition, Wiley-Blackwell (2006).
2. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, 3<sup>rd</sup> edition, Oxford University Press, Oxford (1997).
3. Quantum Chemistry, H. Eyring, J. Walter and G.E. Kimball, (1944) John Wiley, New York.
4. Quantum Chemistry, I.N. Levine, 5th edition (2000), Pearson Educ., Inc., New Delhi.
5. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure, A. Szabo and N. S. Ostlund, (1982), Dover, New York.

**Course Title: Material Chemistry**

**Paper Code: CHM.615**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	0	0	4	100

**Unit I: Metal Oxide**

**18 Hours**

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

**Glasses, Ceramics, Composites and Nanomaterials**

Glassy state, glass formers and glass modifiers, applications. Ceramic structures, mechanical properties, clay products. Microscopic composites; dispersion-strengthened and particle-reinforced, fibre-reinforced composites, macroscopic composites, Nanocrystalline phase, preparation procedures, special properties, applications.

**Unit II: Liquid Crystals and Thin Films**

**24 Hours**

**Liquid Crystals:** 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 III: Polymeric and Ionic Conductors**

**12 Hours**

**Ionic Conductors:** 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 IV: Carbon Materials and NLO Materials**

**18 Hours**

**Fullerenes, Carbon Nanotubes and Graphene (5 hours):** Types and Properties, Methods of

Preparation and separation of carbon nanotubes, applications of fullerenes, CNTs and graphene.

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

**SUGGESTED READINGS**

1. Solid State Physics, N.W. Ashcroft and N.D. Mermin, Saunders College.
2. Material Science and Engineering, An Introduction, W.D. Callister, Willey.
3. Principle of the Solid State, H.V. Keer, Willey Eastern.
4. Material Science, J.C. Anderson, K.D. Leaver, J.M. Alexander and R.D. Rawlings, ELBS
5. Thermotropic Liquid Crystals, Ed., G.W. Gray, John Willey

### SEMESTER 4

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	Weightage				E
								A	B	C	D	
<b>Opt any two courses with one course each from the following optional courses</b>												
1	CHM.616	Bio-inorganic Chemistry	EC	4	1	-	4	25	25	25	25	100
	CHM.617	Advanced Organic Synthesis										
	CHM.618	Medicinal Chemistry- I										
	CHM.619	Quality Control in Laboratory										
	CHM.620	Colloids and Interfaces										
	CHM.621	Statistical Mechanics										
2	CHM.622	Chemistry of Natural Products	EC	4	1	-	4	25	25	25	25	100
	CHM.623	Organotransition Metal Chemistry										
	CHM.624	Molecular Reaction Dynamics										
	CHM.625	Medicinal Chemistry-II										
3	CHM.626	Dissertation Research		-	-	-	16	25	25	25	25	400
		<b>Total</b>		<b>24</b>	<b>2</b>		<b>24</b>					<b>600</b>

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

**A:** Continuous Assessment: Subjective by enlarge

**B:** Mid-Term Test-1: Based on Objective Type & Subjective Type Test

**C:** Mid-Term Test-2: Based on Objective Type & Subjective Type Test

**D:** End-Term Exam (Final): Based on Objective Type Tests

**E:** Total Marks

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

**Course Title: Bio-inorganic Chemistry**

**Paper Code: CHM.616**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

### **Unit 1**

**20 Hours**

#### **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**

**22 Hours**

#### **Inorganic Chemistry of Enzymes - II**

Respiration and photosynthesis; ferridoxins, and subredonim carboxypeptidase, carbonic anhydrase, metallothioneins. Blue copper proteins, superoxide dismutase hemocyanines photosynthesis, chlorophyll and photosynthetic reaction center.

**Enzymes:** Structure and function, inhibition and poisoning Vitamin B12 and B12 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**

**14 Hours**

#### **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**

**10 Hours**

#### **Inorganic Medicinal Chemistry**

Fundamentals of Toxicity and Detoxification. Nuclear medicines

#### **ESSENTIAL BOOKS:**

1. Huheey, J. E., Keiter, E. A. and Keiter, R.L. *Inorganic Chemistry Principles of Structure and Reactivity*, 4th edition, Haper Collins.
2. Douglas, B., McDaniel, D. and Alexander, J. *Concepts and Models of Inorganic Chemistry*, John Wiley and Sons, 3rd edition.
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*, VCH, 2nd edition.
5. Shriver, D.F. and Atkins, P.W. *Inorganic Chemistry*, Oxford University Press, 3rd edition.
6. Cowan, J.A. *Inorganic Biochemistry*, Wiley – VCH, 2nd edition.
7. Lippard, S. J. *Progress in Inorganic Chemistry*, Vols. 18 and 38, Wiley-Interscience, 1991.

**Course Title: Advance Organic Synthesis**

**Paper Code: CHM.617**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Unit 1** **14 hours**

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

**Unit 2** **18 hours**

**Reaction of ylides:** Phosphorus ylide; Structure and reactivity, stabilized ylides, effects of ligands on reactivity, Wittig, Wittig-Horner and Wadsworth, Emmons reactions-mechanistic realization; E/Z selectivity for olefin formation, Schlosser modification: Peterson's olefin synthesis. Sulphur Ylides; Stabilized and non-stabilized ylides: Thermodynamically and kinetically controlled reactions with carbonyl compounds, regio- and stereo-selective reactions

**Unit 3** **20 hours**

**Organometallic compounds**

Organoboranes: Preparation of Organoboranes viz hydroboration with BH<sub>3</sub>-THF, dicyclohexyl borane, disiamyl borane, teryl borane, 9-BBN and disopinacamphyl borane, functional group transformations of Organo boranes-Oxidation, protonolysis and rearrangements. Formation of carbon-carbon-bonds viz organo boranes carbonylation.

Grignard reagents, Organo lithium, Organo zinc, Organo cadmium and Organo Copper Compounds, Organo silicon compounds for organic synthesis, Organopalladium and organostannous (Applications in coupling reactions).

**Unit 4** **20 hours**

**Reagents in organic synthesis:** Gilman's reagent, Lithium diisopropylamide (LDA), Dicyclohexyl Carbodiimide (DCC), 1,3-Dithiane (Umpolung reagent), Trimethylsilyliodide, Baker's yeast, DDQ, Lead tetraacetate, Prevost Hydroxylation, Wilkinson's catalyst, Phase transfer catalysts: Quaternary ammonium and Phosphonium salts, Crown ethers, Merfield resin, Fenton's reagents, Ziegler-Natta catalyst, Lawson reagents, K-selecteride and L-selecteride, Sodium cyanoborohydride, 9-BBN, IBX, Manganese dioxide, Fetizon reagent, Dioxiranes, Ceric ammonium nitrate, Tebbe reagent, Corey-Nicolaou reagent, Mosher's reagent, use of Os, Ru, and Tl reagents.

**ESSENTIAL BOOKS:**

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

3. Finar, I.L., (2012). *Organic Chemistry*, Pearson Education, 6<sup>th</sup> edition, UK.
4. Li, J.J., (2009). *Name Reactions: A Collection of Detailed Reaction Mechanism*, Springer, 4<sup>th</sup> edition.
5. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
6. Reich, H.J., Rigby, M., (1999). *Handbook of Reagents for Organic Synthesis Acidic and Basic Reagents Vol. IV* Wiley-Interscience
7. Warren, S., (2010). *Organic synthesis: The Synthon Approach*. John Wiley & Sons, New York,
8. Warren, S., (2010). *Designing organic synthesis: A Disconnection Approach*. John Wiley & Sons, New York.
9. Corey E.J., Cheng Xue-Min, *The Logic of Chemical Synthesis*, Pubs: John Wiley & Sons, (1989).
10. Fuhrhop Jurgen, Penzlin Gustav, *Organic Synthesis: Concepts methods, Starting Materials*, Pubs: Verlag chemie, (1994).
11. Stuart Warren, *Organic Synthesis: The Disconnection Approach*, Pubs: John Wiley & sons (1982).
12. Davies Stephen G., *Organotransition Metal Chemistry: Application to Organic Synthesis*, Pubs: Pergamon Press (1994).
13. Morrison J. D. (eds) *Asymmetric Synthesis*, Vol. 1 to 5, Pubs: Academic Press. (1992).
14. Aitken R.A. and Kilenyi S.N., *Asymmetric Synthesis*, Pubs: Academic Press. (1994).
15. Proctor Garry, *Asymmetric Synthesis*, Pubs: Academic Press (1996)

**Course Title: Medicinal Chemistry I**

**Paper Code: CHM.618**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

### Unit 1

**18 Hours**

**Physicochemical and stereochemical aspects:** In relation to biological activity, Drug receptor interaction, Adrenergic hormones and Drugs including biosynthesis, storage, release and metabolism of catecholamines (Adrenaline, Isoprenaline, Salbutamol, Amphetamine, Naphazoline), Cholinergics and Anticholinesterases including biosynthesis, storage and metabolism of acetylcholine (Methacholine Chloride, Neostigmine Bromide), Antispasmodic and Antiulcer Drugs (Cyclopentolate, Propantheline Bromide, Benzhexol), Antiparkinsonism Drugs (Apomorphine).

### Unit 2

**18 Hours**

**Neuromuscular blocking agents:** Gallamine Triethiodide, Succinylcholine chloride, Hypoglycaemic drugs (Tolbutamide), Thyroid hormones and Antithyroid drugs (L-Thyroxine, Propylthiouracil).

**Anticoagulants and haemostatic agents:** Warfarin, Phenindione, Oxytocics (includes discussion on Ergot alkaloids) (Ergometrine).

**Antihistamines** including discussion on Sodium cromoglycate (Mepyramine, Diphenhydramine, Chlorpheniramine, Promethazine).

**Non-steroidal anti-inflammatory drugs and anti-gout drugs:** Indomethacin, Phenylbutazone, Allopurinol, Probenecid.

### Unit 3

**18 Hours**

**General Anaesthetic Agents:** Introduction, medicinal aspects of anaesthetics, mode of action, gases and volatile liquid anaesthetics, intravenous anaesthetics or fixed anaesthetics, toxicity of general anaesthetics (Divinyl ether, Ethyl chloride, Cyclopropane, Thiopentone Sodium).

**Local Anaesthetic Agents:** Introduction, Structure-activity relationships, benzoic acid derivatives, aminobenzoic acid derivatives, lidocaine derivatives, miscellaneous, toxicity, mode of action (Benzocaine, Procaine Hydrochloride, Lidocaine Hydrochloride, Ainchocaine Hydrochloride).

### Unit 4

**18 Hours**

**Sedatives-Hypnotics:** Introduction, classification of sedative-hypnotics, structure-activity relationships, barbiturates, amides and imides, alcohols and their carbamate derivatives, aldehydes and their derivatives, mode of action, pharmacological properties and side effects (Barbitone, Phenobarbitone, Cyclobarbitone, Pentobarbitone Sodium, Thiopentone Sodium), non-barbiturates (Official drugs).

**Anticonvulsants:** Introduction, epilepsy and its types, SAR, barbiturates (official products), hydantoin, Oxazolidinediones, Succinamides; miscellaneous drugs, (Phenytoin Sodium, Troxidone).

**Suggested Readings:**

1. Delgado, J. N. and Remers W A, Ed. (2010). *Wilson & Gisvold's Textbook of Organic and Pharmaceutical Chemistry*, J. Lippincott Co., Philadelphia.
2. Foye, W. C. (2008). *Principles of Medicinal Chemistry*, Publisher: Lea & Febiger, Philadelphia.
3. King, F. D. (2006). *Medicinal Chemistry Principles and Practice*, Royal Society of Chemistry, 2<sup>nd</sup> edition, London.
4. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, 3<sup>rd</sup> edition, UK.
5. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*, Oxford University Press, 4<sup>th</sup> edition, US.
6. Singh, H., Kapoor, V.K. (Latest Edition). *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.
7. Smith, H.J. (2006). *Introduction to the Principles of Drug Design and Action*, Taylor and Francis, 4<sup>th</sup> edition.
8. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier).
9. Wolff, M E, Ed., (2010). *Burger's Medicinal Chemistry and Drug Discovery* John Wiley & Sons, 7<sup>th</sup> edition, New York.

**Course Title: Quality Control in Laboratory**

**Paper Code: CHM.619**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Unit I: Introduction 18 Hours**

Concept of Total Quality Management, philosophy of GMP's and GLPS, ISO 9000 and ISO 14798(NABL Accreditation).

Organization and personnel, responsibilities, training, hygiene, personnel records.

Premises: location, design, plan layout, construction, maintenance of sterile areas, control of contamination.

Equipment, selection purchase specifications, preventive maintenance of equipment, cleaning of equipment.

Raw materials: purchase specifications stores selection of vendors, control on raw materials. Warehousing, good warehousing practices, materials management.

**Unit II: Statistical Methods 18 Hours**

**Statistical methods in chemical analysis:** Types of errors, propagation of errors, statistical treatment of random errors, sample and population, Normal distribution, Tests of Significance and Confidence Limits. Method of Least squares and weighted least squares formalism. Use of certified reference materials and procedures for interlaboratory comparisons. Definition of limits of detection and sensitivity, and concept of standard addition to assess matrix effects. Uncertainty Calculations.

**Unit III: Quality Control and GLP 18 Hours**

Quality control laboratory, responsibilities, good laboratory practice, routine controls, instruments reagents, sampling plans, standard test procedures, protocols, non-clinical testing, controls on animal house, data generation and storage, quality control documentation, retention samples, records. Complaints and recalls, evaluation of complaints, recall procedures, related records and documents.

**Unit IV: Regulatory and Validation 18 Hours**

Regulatory aspects of pharmaceutical and bulk drug manufacture. DRA, FDA, CPMP, ICH guidelines.

Regulatory Aspects of Environmental and Food Testing USEPA, MoEF, MoFPI, AOAC guidelines.

Validation: Qualification (IQ/PQ/OQ), validation and calibration of equipment's, Evaluation of Analytical data.

Drug approval process, patent application and WHO certification.

**Suggested Readings**

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

**Course Title: Colloids and Interfacial Surfaces**

**Paper Code: CHM.620**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Unit I: Introduction to Colloids and Interfaces**

**18 Hours**

**Introduction:** Colloids and interface: classification, Colloids - Definition of colloid, properties of lyophilic and lyophobic colloids, stability of colloids, protective action of lyophilic colloids, gold number, definition of gel and emulsion preparation and purification of colloids; Two Fundamental Forces in Surface and Colloid Chemistry Van der Waals, Electrostatic double layer, Acid-base interactions including hydrophobic attraction and hydration pressure.

**Mesoscale thermodynamics:** Gibbs treatment of interfaces; concept of excess concentration; variation of interfacial tensions with surfactant concentration.

Kinetic theory of colloidal systems: sedimentation, centrifugation, diffusion, Brownian movement.

Thermodynamics of surfaces: Gibbs adsorption isotherm, heat and entropy of adsorption.

**Unit II: Physical Aspects of Interfaces and Colloids**

**18 Hours**

Surface film on liquids; Electro-kinetic phenomena.

Surface energy: surface tension, Laplace equation, wetting - capillarity - adhesion - cohesion - dispersion, porosimetry, illustrations.

**Properties of charged surfaces:** origin of charge, physical and chemical models of the double layer, interactions between particles and stability of colloidal systems electrical properties – charge, electrical double layer; DVLO theory, electrokinetic properties: electrophoresis, electroosmosis; Analysis of surface charge and surface chemistry (electrokinetics [electrophoresis, streaming potential, electro-osmosis, sedimentation potential], electroacoustics, surface spectroscopy, ESR)

Optical and Physical properties, determination of size of colloidal particles involving microscopy, scattering (ILS, DLS, x-ray, neutron), sedimentation, centrifugation, chromatography, acoustics, adsorption. Interphase region, curved surfaces.

**Unit III: Surfactants and Micelles**

**18 Hours**

Surface active agents, classification of surface active agents, micellization, micelle structure and shape, shape transitions, elongated micelles, vesicles, inverted structures, micelle aggregation number, hydrophobic interaction, critical micelle concentration (CMC), factors affecting the CMC of surfactants, counterion binding to micelles, thermodynamics of micellization,  $\Delta G$ ,  $\Delta H$ ,  $\Delta S$  of micelle formation, phase separation, and mass action models, solubilization, microemulsion, nanoemulsions, reverse micelles. Gemini surfactants.

**Unit IV: Applications of Colloids**

**18 Hours**

Micellar catalysis, drug formulation and drug delivery, Superhydrophobicity, Applications in wastewater/water treatment, and oil field.

**Adsorption and Catalysis:** Bimolecular surface reactions-reaction between a gas molecule and adsorbed molecule, reaction between two adsorbed molecules, inhibition and activation energy of such reactions. Catalytic activity at surfaces, transition state theory of surface reactions: rates of chemisorption and desorption, unimolecular and bimolecular surface

reaction, comparison of homogeneous and heterogeneous reaction rates, surface heterogeneity, lateral interaction.

**Books:**

1. Principles of Colloid and Surface Chemistry, Paul C. Hiemenz, Marcel Dekker, any edition starting with the 2nd edition, 1986.
2. Physical Chemistry of Surfaces, Arthur W. Adamson, 5th edition, Wiley, 1990.
3. Foundations of Colloid Science, Robert J. Hunter, Clarendon, Oxford, Volume 1, 1989.
4. Colloidal Dispersions, W. B. Russel, D. A. Saville and W. R. Schowalter, Cambridge University Press, 1989.
5. Intermolecular and Surface Forces, Jacob N. Israelachvili, Academic Press, 1992 or later editions.
6. Interfacial Forces in Aqueous Media, Carel J. van Oss, Marcel dekker or Taylor & Francis, 1994.

**Course Title: Statistical Mechanics**

**Paper Code: CHM.621**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Course objective:** The objectives of this course are to develop and understanding of the statistical nature of the laws of thermodynamics, to examine the basic theory of statistical mechanics and to apply this theory to a wide variety of interesting problems.

**Unit 1** **18 Hours**

**Ensemble:** Microcanonical, canonical and grand canonical ensemble; ensemble averages, most probable distributions, thermodynamic connections and fluctuations.

**Unit 2** **18 Hours**

**Classical Statistical Mechanics:** Classical partition function, Phase space and the Liouville theorem, Equipartition of energy.

**Unit 3** **20 Hours**

**Bose-Einstein and Fermi-Dirac distributions:** Special case of Boltzmann statistics, FD and BE statistics, weakly and strongly degenerate ideal gases, Blackbody radiations, Einstein condensation. The density matrix and quantum mechanical analog of the Liouville equation.

**Unit 4** **16 Hours**

**Crystals and Imperfect Gases:** Vibrational spectrum of monatomic crystals, Einstein theory of specific heat of crystals, Debye theory of heat capacity of crystals. Virial equation of state, virial coefficients, law of corresponding states.

#### **ESSENTIAL BOOKS:**

1. D. A. McQuarrie, *Statistical Mechanics*, California University Science Books (2000).
2. R.H. Swendsen, *An Introduction to Statistical Mechanics and Thermodynamics* (Oxford University Press, Oxford, U.K.) (2012).
3. R.K. Patharia and Paul D. Beale, *Statistical Mechanics* (Elsevier, USA) (2011).
4. B.B. Laud, *Fundamentals of Statistical Mechanics* (New Age International, New Delhi, India) (2012).
5. K. Huang, *Statistical Mechanics* (Wiley India Pvt. Ltd., New Delhi, India) (1987).
6. F. Reif, *Fundamentals of Statistical and Thermal Physics*, McGraw-Hill (1965).
7. L.D. Landau and E.M. Lifshitz, *Statistical Physics*, 3<sup>rd</sup> edition, Pergamon (1980).

**Course Title: Chemistry of Natural Products**

**Paper Code: CHM.622**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Unit 1** **18 hours**

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

**Unit 2** **18 hours**

**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 hours**

**Steroids:** Occurrence, nomenclature, basic skeleton and stereochemistry, Structure determination and synthesis of cholesterol, partial synthesis of Testosterone and Progesterone, Chemical tests for steroids

**Unit 4** **9 hours**

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

**Unit 5** **9 hours**

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

**Suggested Readings:**

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

**Course Title: Organotransition Metal Chemistry**

**Paper Code: CHM.623**

**Total Lectures: 72**

L	T	P	Credits	Marks
4	1	0	4	100

### **Unit 1**

**18 Hours**

#### **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

#### **Transition Metal Compounds with Bonds to Hydrogen**

Transition metal Compounds with bonds to hydrogen

### **Unit 2**

**18 Hours**

#### **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.

### **Unit 3**

**18 Hours**

#### **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 Hours**

#### **Homogeneous Catalysis**

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

#### **ESSENTIAL BOOKS:**

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

**Course Title: Molecular Reaction Dynamics**

**Paper Code: CHM.624**

**Total Hours: 72**

L	T	P	Credits	Marks
4	1	0	4	100

**Unit 1**

**18 Hours**

**Potential Energy Surfaces:** Long-range Potentials, Empirical Intermolecular Potentials, Molecular Bonding Potentials, Internal Coordinates and Normal Modes of Vibration, Ab Initio Calculation of Potential Energy Surfaces, Analytic Potential Energy Functions, Details of the Reaction Path.

**Unit 2**

**18 Hours**

**Dynamics of Bimolecular Collisions:** Simple Collision Models, Two-Body Classical Scattering, Complex Scattering Process.

**Unit 3**

**18 Hours**

**Transition State Theory:** Basic Postulates and Derivation of Transition State Theory, Dynamical Derivation of Transition State Theory, Quantum Mechanical Effects in Transition State Theory, Thermodynamic Formulation of Transition State Theory, Applications of Transition State Theory.

**Unit 4**

**18 Hours**

**Unimolecular Reaction Dynamics:** The Lindmann-Hinshelwood Mechanism, Statistical Energy-dependent Rate Constant, RRKM Theory, Applications of RRKM Theory to Thermal Activation.

**ESSENTIAL BOOKS:**

1. J. I. Steinfeld, J. S. Francisco, and W. L. Hase, Chemical Kinetics and Dynamics, Prentice Hall (1998).
2. R. D. Levine, Molecular Reaction Dynamics, Cambridge University Press (2009).
3. N. E. Henriksen F. Y. Hansen, Theories of Molecular Reaction Dynamics: The Microscopic Foundation of Chemical Kinetics, Oxford University Press, USA (2012).
4. M. Brouard, Reaction Dynamics, Oxford Chemistry Primers (1998).
5. P. L. Houston, Chemical Kinetics and Reaction Dynamics, Dover Publications (2012).
6. S. K. Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer (2006).
7. K. J. Laidler, Chemical Kinetics, Pearson (2008).
8. A. H. Zewail, Femtochemistry-Ultrafast Dynamics of the Chemical Bond, World Scientific, New Jersey (1994).

**Course Title: Medicinal Chemistry-II**

**Paper Code: CHM.625**

**Total Hours: 72**

L	T	P	Credits	Marks
4	1	0	4	100

### **Unit 1**

**18 Hours**

**Steroids:** Introduction, nomenclature, stereochemistry of cholesterol, stigmasterol, ergosterol, diosgenin, solasodine, bile acids, biosynthesis of testosterone,  $\beta$ -estradiol and aldosterone from cholesterol, Estrogens, SAR among estrogens, progestational agents, synthesis of progesterone from diosgenin and stigmasterol, ethisterone from dehydroepiandrosterone, oral contraceptives, SAR of progestins, Androgens and Anabolic Agents: Synthesis of testosterone from diosgenin, methyltestosterone from dehydroepiandrosterone, methandienone from methyl testosterone, stanozolol from testosterone. Adrenocorticoids: Glucocorticoids and their SAR, mineralocorticoids, modifications in structure of hydrocortisone.

### **Unit 2**

**18 Hours**

**Opioid analgesics:** Morphine and related drugs, synthetic modifications of morphine, codeine and thebaine, synthetic analgesics, endogenous opioid peptides, opioid antagonists, CNS stimulants, natural and synthetic, Methylxanthines and modified Methylxanthines, Psychopharmacological agents, Antipsychotics, Phenothiazines, Antidepressants: Tricyclic antidepressants, MAO inhibitors, atypical antidepressants, Antianxiety drugs: Meprobamate and related drugs, Benzodiazepines, Hallucinogens Hallucinogenic agents related to indoles, phenethylamines and Cannabinoids.

### **Unit 3**

**18 Hours**

**Diuretics carbonic anhydrase inhibitors:** Thiazides and related drugs, High-ceiling diuretics. Aldosterone, antagonists, Other potassium sparing diuretics, Osmotic diuretics, Cardiovascular Agents: cardiac glycosides, SAR, mechanism of action, toxic effects. Antihypertensive agents; introduction, ganglion blocking agents, antiadrenergic agents, drugs acting directly on smooth muscles, drugs acting on CNS. Antianginals and vasodilators: introduction, mechanism of smooth muscle vasodilation, esters of nitrous and nitric acid, side-effects. Antiarrhythmic and antifibrillatory drugs classification of antiarrhythmic drugs, mechanism of action, side effects. Antilipemic drugs.

### **Unit 4**

**18 Hours**

**Sulphonamides:** Introduction and classification, antimicrobial spectrum, DHFR inhibitors, toxicity and side effects, reduction. Antibiotics: Classification, cycloserine, chloramphenicol, penicillins, cephalosporins, aminoglycosides, tetracyclines, polypeptides. Antimycobacterial agents: Introduction, uses in therapeutics. Antimalarials: quinoline and analogues, 8-amino quinolines, 9-amino acridines, 4-amino quinolines, diamino pyrimidine, and biguanides and recently introduced compounds. Antiamoebic agents; quinoline derivatives, metal free substances, diloxanide furoate, etc. Anthelmintic drugs in cestode infections in trematode infections and for intestinal nematode infections, antifilarial agents, Antiviral agents:

Introduction to DNA, RNA and retroviruses, viral application, amantidine hydrochloride, interferones, acyclovir, idoxuridine, trifluorothymidine and vidarabine etc.

**Suggested Readings:**

1. Delgado, J. N. and Remers W A, Ed. (2010). *Wilson & Gisvold's Textbook of Organic and Pharmaceutical Chemistry*, J. Lippincott Co., 7<sup>th</sup> edition, Philadelphia.
2. Foye, W. C. (2008). *Principles of Medicinal Chemistry*, Publisher: Lea and Febiger, 6<sup>th</sup> edition, Philadelphia.
3. King, F. D. (2003). *Medicinal Chemistry Principles and Practice*, Royale Society of Chemistry, 2<sup>nd</sup> Edition, London.
4. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, 3<sup>rd</sup> edition, New York.
5. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*, Oxford University Press, 4<sup>th</sup> edition. UK.
6. Singh, H., Kapoor, V.K. (Latest Edition). *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.
7. Smith, H.J. (2006). *Introduction to the Principles of Drug Design and Action*, Taylor and Francis, 4<sup>th</sup> edition, UK.
8. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier), 3<sup>rd</sup> edition.
9. Wolff, M E, Ed., (2010). *Burger's Medicinal Chemistry and Drug Discovery*, John Wiley and Sons, New York.

**Course Title: Dissertation Research**  
**Paper Code: CHM.626**

L	T	P	Credits	Marks
-	-	-	16	400