

**For Batches 2015 & Onwards**  
Academic Autonomous Institute (No. F22-1/2014 (AC))

Beant College of Engineering & Technology,  
Gurdaspur

**STUDY SCHEME & SYLLABUS  
OF  
M.Sc. (CHEMISTRY)**

BCET

**For Batches 2015 & Onwards**  
Academic Autonomous Institute (No. F22-1/2014 (AC))

**Semester-I**

**(Max. Marks: 900)**

Course Code	Course Title	Load Allocation			Marks Distribution		Credits
		L	T	P	Internal	External	
<b>MSCH-101</b>	Inorganic Chemistry-I	3	1	-	50	100	4
<b>MSCH-102</b>	Organic Chemistry-I	3	1	-	50	100	4
<b>MSCH-103</b>	Basic Biological Chemistry/Mathematics in Chemistry	3	1	-	50	100	4
<b>MSCH-104</b>	Physical Chemistry	3	1	-	50	100	4
<b>MSCH-105</b>	Inorganic Chemistry Lab-I	-	-	4	50	100	2
<b>MSCH-106</b>	Organic Chemistry Lab-I	-	-	4	50	100	2
<b>Total</b>		<b>12</b>	<b>4</b>	<b>8</b>	<b>300</b>	<b>600</b>	<b>20</b>

**Semester-II**

**(Max Marks: 900)**

Course Code	Course Title	Load Allocation			Marks Distribution		Credits
		L	T	P	Internal	External	
<b>MSCH-201</b>	Organic Chemistry-II	3	1	0	50	100	4
<b>MSCH-202</b>	Symmetry and Group Theory	3	1	0	50	100	4
<b>MSCH-203</b>	Spectroscopy-I	3	1	0	50	100	4
<b>MSCH-204</b>	Quantum Chemistry	3	1	0	50	100	4
<b>MSCH-205</b>	Physical Chemistry Lab	0	0	4	50	100	2
<b>MSCH-206</b>	Organic Chemistry Lab-II	0	0	4	50	100	2
<b>Total</b>		<b>12</b>	<b>4</b>	<b>8</b>	<b>300</b>	<b>600</b>	<b>20</b>

**For Batches 2015 & Onwards**  
Academic Autonomous Institute (No. F22-1/2014 (AC))

**Semester-III**

**(Max. Marks: 900)**

Course Code	Course Title	Load Allocation			Marks Distribution		Credits
		L	T	P	Internal	External	
MSCH-301	Inorganic Chemistry-II	3	1	0	50	100	4
MSCH-302	Spectroscopy-II	3	1	0	50	100	4
MSCH-303	Computational Skills and Simulations in Chemistry	3	1	0	50	100	4
MSCH-XXX	Elective-I	3	1	0	50	100	4
MSCH-304	Inorganic Chemistry Lab-II	0	0	4	50	100	2
MSCH-305	Computational Skills and Simulations in Chemistry Lab	0	0	4	50	100	2
MSCH-306	Project phase 1	0	0	4	Satisfactory/ Unstatisfactory		
<b>Total</b>		<b>12</b>	<b>4</b>	<b>8</b>	<b>300</b>	<b>600</b>	<b>20</b>

**Semester-IV**

**(Max. Marks: 900)**

Course Code	Course Title	Load Allocation			Marks Distribution		Credits
		L	T	P	Internal	External	
MSCH-401	Dissertation	-	-	-	-	450	8
MSCH-402	Environmental Chemistry	3	1	0	50	100	4
MSCH-403	Analytical Principles and Instrumental Method of Analysis	3	1	0	50	100	4
MSCH-YYY	Elective-II	3	1	0	50	100	4
<b>Total</b>		<b>15</b>	<b>5</b>	<b>8</b>	<b>150</b>	<b>750</b>	<b>20</b>

\* The evaluation of the Project Phase-I is based on the presentation of individual student about the progress report.

**Elective-I** MSCH 311 Polymers, MSCH 312 Medicinal Chemistry

**Elective-II** MSCH 411 Nanochemistry, MSCH 412 Photochemistry

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## **First Semester**

**MSCH-101**  
**INORGANIC CHEMISTRY - I**

**External Marks: 100**  
**Internal marks: 50**  
**Total marks: 150**

**L T P**  
**3 1 0**

**LEARNING OBJECTIVES:**

1. To understand Principles of Molecular Orbital Theory and VSEPR theory completely.
2. To acquire full knowledge of main group chemistry and group 12 elements.
3. To know the structures of ionic solids.
4. To develop an understanding of the inorganic chemistry of elements with respect to their oxidation and reduction.

**UNIT-I**

**1. PRINCIPLES:** Molecular structure and bonding. A review of Lewis structures including formal charges and VSEPR model. Molecular orbital theory of homo- and heteronuclear diatomic molecules. Molecular orbital theory of solids. Periodicity and related concepts. Chemical forces. (07)

**UNIT-II**

**2. CHEMISTRY OF s-BLOCK METALS:** Hydrides, halides, oxides, peroxides, superoxides, suboxides, hydroxides, oxoacid salt complexes, crowns and crypts of alkali metals and coordination complexes of alkaline earth metals. (10)

**UNIT-III**

**3. CHEMISTRY OF p-BLOCK ELEMENTS:** Boranes, bonding in boranes, topology of boranes, synthesis and reactivity. Carboranes and metallocarboranes, borazine and boron nitride. Chemistry of aluminum halides, aluminum alkyls. Low oxidation state aluminium compounds. Organosilicon compounds. Silicates and aluminosilicates. Low-valent silicon compounds, silylenes and  $R_3Si^+$ , Polysilanes. Phosphazenes, cyclophosphazenes, polyphosphazenes and the polymers derived from them. (10)

**4. CHEMISTRY OF GROUP 12 ELEMENTS:** Halides & oxygen compounds, chalcogenides & related compounds, low-valent compounds. Formation of coordination complexes. (05)

**UNIT-IV**

**5. SOLID STATE:** Close-packing of solids, types and structures of ionic solids; radius ratio rules; lattice energy; Born-Haber cycles, defects in solids and properties of solids arising out of defects in structures, Perovskite structures, high  $T_c$  superconductors. (07)

**6. OXIDATION AND REDUCTION:** Reduction potentials, redox stability in water, diagrammatic presentation of potential data, acids and bases, Various definitions including HSAB principles, Thermodynamic acidity parameters, solvents as acids and bases. (06)

**INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

1. Examiner will set total of **NINE** questions comprising **TWO** questions from each unit and **ONE** compulsory question of short answer type covering whole syllabus.

2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question. 3. All questions carry equal marks.

**BOOKS RECOMMENDED:**

1. W. Henderson, **Main Group Chemistry**, Royal Society of Chemistry, UK, 2000.
2. J. E. Huheey et. al, **Inorganic Chemistry, Principles of Structure and Reactivity**, Fourth edition, Pearson Education, India, 2006.
3. J. D. Lee, **Concise Inorganic Chemistry**, Fifth edition, Wiley India Pvt, Ltd. 2008.
4. Norman Greenwood, Andrew Hughes, Mark Fox, Keith Dillon, Kenneth Wade, **Chemistry of Elements**, Elsevier, 2011.
5. Peter Atkins, Tina Overton, **Shriver and P. W. Atkins' Inorganic Chemistry**, 5th edition Oxford University Press, Oxford, 2009.
6. F. Albert Cotton, Carlos A. Murillo, Manfred Bochmann, Russell N. Grimes, **Advanced Inorganic Chemistry**, 6th edition, Wiley-Interscience, 1999

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**MSCH-102**  
**ORGANIC CHEMISTRY - I**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**3 1 0**

**LEARNING OBJECTIVES:**

1. To understand different types of organic synthesis.
2. To understand use of various reagents in organic synthesis.
3. To understand asymmetric synthesis and characterize the compounds synthesized.

**UNIT - I**

General Introduction to organic synthesis, types of organic synthesis: retrosynthesis, disconnection, Linear and convergent synthesis, synthons, synthetic equivalents, umpolung of reactivity and protective groups, protection and deprotection of general functional groups, functional group interconversions, applications of green chemistry to organic synthesis. (12)

**UNIT - II**

Use of following reagents in Organic synthesis and functional group transformations; compounds of Mg, Li, Cu, B, Si and P in organic synthesis, Gilman's reagent, lithium diisopropylamide (LDA), dicyclohexylcarbodiimide (DCC), 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), trimethylsilyl iodide, tri-n-butyltin hydride, osmium tetroxide, selenium dioxide. Phase transfer catalysts, crown ethers and Merrifield resin, Wilkinson's catalyst, Baker yeast, ionic liquids, water. (11)

**UNIT - III**

Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction-substrate, reagent and catalyst controlled reactions, determination of enantiomeric purity by GC, HPLC, NMR etc., enantio-discrimination, resolution- optical and kinetic, chiral phase transfer catalysis, chiral quaternary ammonium salts, asymmetric proton catalysis, asymmetric acyl transfer reactions. (11)

**UNIT - IV**

General methods of preparation and reactions of indene, fluorine, anthracene and phenanthrene, three-membered, four-membered, five-membered and six-membered heterocyclic compounds: synthesis and reactions of oxiranes, thiiranes, azetidines, aziridines, oxetanes, thietanes, pyrrole, pyrrolidine, furan, tetrahydrofuran, pyrylium salts, pyrones, pyridinium and thiopyrylium salts, pyridones, quinolinium and benzopyrylium salts, coumarins and chromones. (11)

**INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

1. Examiner will set total of **NINE** questions comprising **TWO** questions from each unit and **ONE** compulsory question of short answer type covering whole syllabus.
2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks.

**BOOKS RECOMMENDED:**

1. Willis Christine and Wills Martin, **Organic Synthesis**, Oxford University Press, 1995.
2. Corey E.J., X.M. Cheng, **The logic of Chemical Synthesis**, Wiley Interscience, 1995.



3. Thomas S.E., **Organic Synthesis: The roles of Boron and Silicon**, Oxford University Press, 1992.
4. Jenkins Paul R., **Organometallic Reagents in Synthesis**, John Wiley, 1994.
5. Mackie R.K., Smith D.M., **Guide Book to Organic Synthesis**, 2nd edition, Longman, 1995.
6. Acheson R.M., **An Introduction to the Chemistry of Heterocyclic Compounds**, Wiley, 3rd edition, New York, 1976.
7. Michael B. Smith, Jerry March, **March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure**, (6th Edition), Wiley-Interscience, 2007.
8. Carey F.R., Sunberg R.J., **Advanced Organic Chemistry**, 5th edition, Springer, 2007.
9. Davies Stephen G., **Organotransition Metal Chemistry: Applications to Organic Synthesis**, Pergamon Press (1994).
10. Morrison J.D. (eds.), **Asymmetric Synthesis: Vol.1-5**; Academic Press, 1992.
11. Aitken R.A., Kilenyi S.N., **Asymmetric Synthesis**

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**MSCH-103**  
**BASIC BIOLOGICAL CHEMISTRY**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**3 1 0**

**LEARNING OBJECTIVES:**

1. To understand detailed structures of proteins & nucleic acids.
2. To understand role of enzymes.
3. To understand detailed mechanism and functions of carbohydrates.

**UNIT - I**

**1. BIO-MOLECULES:** Broad classification- water, pH, ionization, biological buffers, titration of amino acids. Proteins and their three dimensional structure, weak and strong interactions. Basic structure of carbohydrates (monosaccharide, disaccharides & polysaccharides). Nucleic acids- purines, pyrimidines, nucleosides, nucleotides, internucleotide bonding, tautomerism, lipids, neutral lipids, phospholipids, isoprenoids, phosphatidylinositol, biological effectors. (07)

**2. PROTEINS:** Structural and functional classification of proteins. Structure, physicochemical properties, configuration properties of amino acids. Colour reactions of proteins and amino acids, Purification of proteins and amino acid sequence determination, peptide bond. Ramachandran plot. Primary, secondary tertiary and quaternary structures of proteins. Three dimensional structures of proteins. Structure and functions of hemoglobin. (10)

**UNIT - II**

**3. ENZYMES:** General properties of enzymes and co-enzymes, their nature. Classification and nomenclature of enzymes. Mechanism & kinetics of enzymatic reactions. Michaelis Menton model, enzyme inhibition. Kinetics of competitive and non-competitive enzymatic inhibition. Isozymes allosteric enzymes. Mechanism of enzymatic catalysis by lysozyme and carboxypeptidase. Zymogens. (10)

**UNIT - III**

**4. COENZYMES:** Classification, structure and function of nicotinamide adenine dinucleotides (NAD and NADP), riboflavin nucleotides (FMN and FAD), lipoic acid, cytochromes, pyridoxal phosphate, nucleoside diphosphates, tetrahydrofolic acid conjugates, biotinyl coenzyme, coenzyme - A, thiamine pyrophosphate. (08)

**UNIT - IV**

**5. CARBOHYDRATES AND METABOLISM:** Configuration and chemical transformations and reactions of carbohydrates, Absolute configuration of carbohydrates, general concepts, energetics and control on metabolic pathways. Glycolysis, alcoholic and lactic acid fermentation, citric acid cycle, EDP pathway. Disaccharide and polysaccharide metabolism, gluconeogenesis, regulation of carbohydrate metabolism, electron transport chain, oxidative phosphorylation (10)

**INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

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2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks.

**BOOK RECOMMENDED**

1. L. Stryer, **Biochemistry**, W.H. Freeman & Company, 4th Edition, 1995.
2. D. Voet and J.G. Voet, **Biochemistry**, John Wiley & Sons, 2nd Edition, 1995.
3. Michael D. Trevan, **Immobilized Enzymes: An introduction and application in Biotechnology**, John Wiley, 1980.

BCET

**MSCH-103**  
**MATHEMATICS IN CHEMISTRY**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**3 1 0**

**LEARNING OBJECTIVES:**

1. To understand various methods of numerical solutions of differential equations.
2. To study how to apply regression analysis to probability distribution.
3. To study use of Chi-square, t and F statistics.

**UNIT - I**

**1. SYSTEM OF LINEAR EQUATIONS:** Gauss- elimination method - Crout's method - inverse of a matrix. Iterative methods: Jacobi's method - Gauss-Seidel Method. Numerical differentiation and integration - Newton-Cotes formulae.

**UNIT - II**

**2. NUMERICAL SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS:** Picard's Method, Taylor's series Method, Euler's Method, Modified Euler's method, Runge- Kutta Methods. Numerical solution of partial differential equations: finite difference methods.

**UNIT - III**

**3. CORRELATION ANALYSIS AND REGRESSION ANALYSIS:** Probability-addition and multiplication theorems. Probability distributions: Binomial, Poisson and normal distribution

**UNIT - IV**

**4. ELEMENTARY CONCEPTS IN TESTING OF STATISTICAL HYPOTHESIS:** Tests of significance: tests based on normal distribution, Chi-square, t and F statistics. Analysis of variance: One way classification, two way classifications with one observation per cell.

**INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

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2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks.

**BOOKS RECOMMENDED**

1. Mckean, J.W. and Craig, A.T. Mukhopadhyay, P, **Mathematical Statistics.**
2. Gupta and Kapoor, **Fundamentals of Mathematical Statistics,** Sultan Chand & Sons, 2012.
2. Goon, Gupta and Das Gupta, **Fundamentals of Statistics,** World Press

Private, 2005.

4. S.S. Sastry, **Introductory Methods of Numerical Analysis,** PHI Learning Pvt. Ltd., 4th edition, 2005.
5. Conte and de Boor, **Elementary Numerical Analysis,** McGraw Hill, New York, 1990.
6. John H. Mathews, **Numerical Methods for Mathematics, Science and Engineering,** 2nd Edn., Prentice Hall, New Delhi, 2000.

**MSCH-104**  
**PHYSICAL CHEMISTRY**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**3 1 0**

**LEARNING OBJECTIVES:**

1. To understand the laws of thermodynamics.
2. To study the reaction rates of different order reactions.
3. To study the various aspects of electrochemistry.

**UNIT - I**

**1. THERMODYNAMICS:** Concepts involved in first and second law of thermodynamics, Entropy, chemical potential and free energy . Maxwell's relations, Partial molar properties and their significance. Concept of activity and fugacity and their determination. Nernst heat theorem, third law of thermodynamics.

General introduction : Phase space, microstates, macrostates, thermodynamic probability. Thermodynamic probability and entropy. Brief introduction to different types of statistics (Maxwell - Boltzman, Bose – Einstein and Fermi - Dirac statistics). Ensemble concept. Canonical, grand canonical and microcanonical ensembles. Stirling approximation. Maxwell-Boltzmann statistics. Partition functions: Expressions of translational, rotational, vibrational and electronic and nuclear partition functions. (16)

**UNIT - II**

**2. CHEMICAL KINETICS:** Principle of detailed balancing (simple idea only), Effect of temperature on reaction rates. Collision theory of reaction rates (detailed), preliminary idea of transition state theory, Lindemann theory of Unimolecular reactions. Opposing and consecutive reactions. Static, flow and relaxation methods of measurement of reaction rates. Kinetics of fast reaction. preliminary idea of inner sphere and outer sphere reactions of transition metals.

Homogeneous and heterogeneous catalysis, Michaelis-Menten mechanism for enzyme catalysis, autocatalysis and oscillatory reactions (general introductions only). (10)

**UNIT - III**

**3. ELECTROCHEMISTRY:**

Mean ionic activity co-efficient of electrolyte. Debye – Huckel theory. Precise determination of dissociation constants of weak electrolytes – emf and conductometric method. Debye Huckel theory of strong electrolytes, Onsagar conductance equation. Irreversible electrode processes: Polarography and overvoltage. Polarographic cell assembly, merits of dropping mercury electrode. Basic principle of cyclic voltametry and coulometry only. (10)

## UNIT - IV

### 4. MISCELLANEOUS TOPICS:

**(a) Molecular Structure:** Dielectric polarization, Debye – Langevin equation, dipole moment determination and applications, intermolecular forces and their contribution to intermolecular potential.

**(b) Fluid Mechanics:** Fundamental principles of fluid mechanics, Newtonian and Non-Newtonian fluids. Stream line and turbulent flow.

**(c) Refractories:** Refractory materials: Nomenclature, classification- acidic, basic and neutral refractories, important properties and uses. (09)

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2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks.

### BOOKS RECOMMENDED:

1. Silbey, Alberty, et.al., **Physical Chemistry**, 4th Edition, Wiley India Pvt. Ltd., 2006.
2. Atkins, P.W., Julio de Paula, **Physical Chemistry**, 8th edition, ELBS, 2006.
3. Chandra, A.K, **Introductory Quantum Chemistry**, 4th edition, Tata McGraw Hill, 2004.
4. Laidler, Keith J., **Chemical Kinetics**, 3rd edition, Harper & Row, Publishers, New York, 1987.
5. Young, R.J; Lovell, P.A., **Introduction to Polymers**, 2nd edition, Chapman and Hall, 1991.
6. Flory, P.J., **Principles of Polymer Chemistry**, 1st edition, Asian Book Private Ltd., 2006.
7. Crow, D.R., **Principles and Applications of Electrochemistry**, 4th edition, Chapman and Hall, London, 1994.

**MSCH-105**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**0 0 4**

**INORGANIC CHEMISTRY LAB-I**

**LEARNING OBJECTIVES:**

1. To know skills of using various glass wares and apparatus and chemicals used in synthetic inorganic chemistry.
2. To improve the environment of the laboratory and health of the students.
3. To know the chemistry principles applied in the qualitative analysis.
4. To understand various techniques of salt analysis.

**1. WORKING IN CHEMISTRY LAB:**

Introduction – Personal protection – Nature of Chemicals – Toxic, Corrosive, Explosive, Inflammable, Carcinogenic, other hazardous chemicals – Safe storing and handling of chemicals – Disposal of chemical wastes – Glassware – Handling of Glassware – Handling of different types of equipments like Bunsen burner, Certifuger, Gibb's Apparatus, etc. – Ventilation facilities – Philosophy of Lab Safety – First-Aid techniques – General work culture inside the chemistry lab.

**2. PREPARATION OF COORDINATION COMPOUNDS, THEIR PURIFICATION BY CHROMATOGRAPHY, ELEMENTAL ANALYSES (M, S, HALOGEN, C, H, N), M.W. DETERMINATION (RAST METHOD) AND ELUCIDATION OF STRUCTURES BY PHYSICAL METHODS (UV, IR, NMR, MAGNETIC SUSCEPTIBILITY):**

- (a) Synthesis of Tris(acetylacetonato)manganese(III),  $Mn(acac)_3$  and their characterization.
- (b) Synthesis and Characterization of Hexamminechromium(III) nitrate  $[Cr(NH_3)_6](NO_3)_3$  using magnetic susceptibility balance (MSB) and infra red spectroscopy IR (Green Preparation).
- (c) Synthesis of Iron(III) dithiocarbamate and its characterization using magnetic susceptibility balance (MSB) and infra red spectroscopy (IR).
- (d) Synthesis and characterization of nitro- and nitritopentamminecobalt (III) chlorides using infra red spectroscopy (IR).
- (e) Synthesis of hexamminecobalt(III) chloride and pentammineaquocobalt(III) chloride.
- (f) Synthesis of cis- and trans- potassiumdioxalatodiaquochromate(III).
- (g) Aquation of trans-dichlorobis(1,2-diaminoethane)cobalt(III) chloride.
- (h) Synthesis and resolution of tris(ethylenediamine)cobalt(II) ion.
- (i) Synthesis of Hexaamminenickel(II) chloride and estimation of Ni(II) in the complex by gravimetry and volumetry.
- (j) Synthesis of tris(acetylacetonato)iron(III).
- (k) Synthesis and reactivity of organocobaloximes.
- (l) Synthesis of acetylferrocene and its purification by column chromatography.
- (m) Synthesis of ferrocene carboxylic acid.

**3. SYNTHESIS OF GREEN REAGENTS:**

Green Chemistry: Introduction, principles of green chemistry, some green reagents.

- (a) Tetrabutylammonium tribromide (TBATB) and its applications.
- (b) Ionic liquid, 1-methyl-3-pentyl-imidazolium bromide,  $[pmlm]Br$  and its applications.

**4. GENERAL PRINCIPLES OF QUALITATIVE ANALYSIS:**

Principle of flame testing – theory of testing acid radicals (simple and interfering). Principle of grouping of cations – theory of testing cations.

**5. INORGANIC ANALYSIS BY USING GREEN METHODS:**

1. Analysis of simple acid radicals: carbonate, sulfide, sulfate, thiosulfite, chloride, bromide, iodide, nitrate.
2. Analysis of interfering acid radicals: fluoride, oxalate, borate, phosphate, arsenate, arsenite.
3. Elimination of interfering acid radicals and identifying the groups of basic radicals.

4. Analysis of basic radicals (group-wise): Lead, copper, bismuth, cadmium, tin, antimony, iron, aluminium, arsenic, zinc, manganese, nickel, cobalt, calcium, strontium, barium, magnesium, ammonium.
5. Repeating the tests in no. 04
6. Repeating the tests in no. 04
7. Analysis of a mixture-I containing three cations and three anions (of which one is interfering type).
8. Analysis of a mixture-II containing three cations and three anions (of which one is interfering type).
9. Analysis of a mixture-III containing three cations and three anions (of which one is interfering type).
10. Analysis of a mixture-IV containing three cations and three anions (of which one is interfering type).

Note: 1. The students must have exposure of at least two analytical instruments.  
Four experiments must be performed from section 2 & 5.

**BOOKS RECOMMENDED:**

1. H. Denny, W. Roesky, **Chemical Curiosities**, WILEY VCH, 1996.
2. G. Marr and B. W. Rocket, **Practical inorganic chemistry**, University Science Books, 1999.
3. G. Pass and H. Sutcliffe, Chapman and Hall, **Practical Inorganic Chemistry**, London, 2nd edition, 1974.
4. J. Mendham, R. C. Denney, J. D. Barnes, M Thomas, **Vogel's Textbook of Quantitative Analysis**, Pearson education, 5th edition, 2006.
5. G. Svehla, **Vogel's Textbook of Quantitative Analysis**, Pearson education, 2006.
6. Anil J. Elias, **A Collection of interesting General Chemistry Experiments**, Orient Longman Limited, Universities Press (India) Pvt. Ltd., 2008.
7. <http://dst.gov.in/green-chem.pdf>



**MSCH-106**  
**ORGANIC CHEMISTRY LAB-I**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**0 0 4**

**1. QUALITATIVE ORGANIC ANALYSIS:**

Separation and purification of components of binary mixture (Solid/solid, solid/liquid and liquid/liquid) on the basis of solubility behaviour and solvent extraction and their identification and conformation by chemical tests and preparation of suitable derivative. Preparative TLC separation for IR and PMR spectral studies of the respective component.

**2. ORGANIC SYNTHESIS:**

Benzoylation : Hippuric acid

Oxidation : Adipic acid/p-Nitrobenzoic acid

Aldol condensation : Dibenzalacetone/Cinnamic acid

Sandmeyer's reaction : p-Chlorotoluene

Benzfused Heterocycles : Benzimidazole

Cannizzaro's reaction : p-Chlorobenzaldehyde as substrate

Friedel Crafts reaction : S-Benzoylpropionic acid

Aromatic electrophilic

substitution : p-Nitroaniline / p-Iodoaniline

The products may be characterized by spectral techniques.

**BOOKS RECOMMENDED:**

1. **Vogels's Textbook of Practical Organic Chemistry**, 5th Edition ELBS (Longman), 1996.
2. F.G. Mann and B.C. Saunders, **Practical Organic Chemistry**, 5th Edition, Orient Longman Limited, 1986.

# BCET

## **Second Semester**

**MSCH-201**  
**ORGANIC CHEMISTRY-II**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**3 1 0**

**LEARNING OBJECTIVES:**

1. To understand principles of stereochemistry.
2. To understand structures of supramolecular chemistry.
3. To understand applications of photochemistry.

**UNIT - I**

**1. PRINCIPLES OF STEREOCHEMISTRY:** Configurational and conformational isomerism in acyclic and cyclic compounds, stereogenicity, stereoselectivity, enantioselectivity and diastereoselectivity. Configurational and conformational effects on reactivity and selectivity/specificity. Elements of symmetry, chirality, molecules with more than one chiral centres, chirality of organic molecules without chiral centres (biphenyls, allenes, spiranes) and due to helical shape. Enantiotopic and diastereotopic atoms, groups and faces. Stereoselective and stereospecific synthesis. (11)

**UNIT – II**

**2. SUPRAMOLECULAR CHEMISTRY:** Nature of supramolecular interactions, pre- organization and complementarity. Classification of supramolecular host-guest compounds- crown ethers, calixarenes, cyclophanes, cryptands, cyclodextrins, fullerenes, micelles and vesicles. Supramolecular reactivity and catalysis, supramolecular photochemistry, molecular machines based on catenanes and rotaxanes. (11)

**UNIT – III**

**3. PHOTOCHEMISTRY:** Basic principles of photochemistry, photochemistry of alkenes, carbonyl compounds, arenes and fullerenes, photooxidation and photoreduction, Organic solid state photochemistry, chemiluminescent reactions, Barton reaction, di-p-methane rearrangement. Principles and applications of photochemical reactions in organic chemistry, pericyclic reactions- electrocyclicization, cycloaddition, sigmatropic rearrangements and related concerted reactions. Applications of pericyclic reactions in synthesis. (11)

**UNIT - IV**

**4. METAL SALT CATALYSIS:** Fundamental reaction steps of transition metal catalysed reaction, oxidative-addition reactions, elimination reactions, cleavage of C-H bonds, migration reaction and insertion reaction. Homo/heterogeneous catalysis by transition metal complexes. Hydrogenation reaction, alkene isomerisation, hydrosilylation and hydroboration reaction, alkene hydrogenation, reaction of CO and hydrogen, hydroformylation of unsaturated compounds, carbonylation reactions, C-C cross coupling and related reactions, reactions of conjugated dienes, reactions of alkynes, alkene and alkyne metathesis, phase transfer catalysis, C-H activation using metal salts, Suzuki reaction, Heck reaction, Negishi coupling, Stille reaction, Sonogashira coupling reactions. (12)

**INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

1. Examiner will set total of **NINE** questions comprising **TWO** questions from each unit and **ONE** compulsory question of short answer type covering whole syllabus.
2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks

**BOOKS RECOMMENDED:**

1. B. Smith, Jerry March, **March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure**, 6th Edition, Wiley-Interscience, 2007.
2. Carey F.R., Sunberg R.J., **Advanced Organic Chemistry**, 5th edition, Springer, 2007.
3. J.W Steed and J.L. Atwood, **Supramolecular Chemistry**, John Wiley & Sons, NY, 2000.
4. E.L. Eliel, S.H. Wilen, **Stereochemistry of Organic Compounds**, Wiley, 1994.
5. P.S. Kalsi, **Stereochemistry: Conformation and Mechanism**, New Age International Edition, 7th Edition, 2009.
6. N.J. Turro, V. Ramamurthy and J.C. Scaiano, **Principles of Molecular Photochemistry, An Introduction**, University Science Books, 2008.
7. W.M. Horspool and P.S.Song (Ed.), **Handbook of Organic Photochemistry and Photobiology**, CRC Press, 1995.

**MSCH-202**  
**SYMMETRY AND GROUP THEORY**

External Marks: 100

Internal marks: 50

Total Marks: 150

L T P  
3 1 0

**LEARNING OBJECTIVES:**

1. To educate students about the importance of symmetry elements and operations.
2. To acquaint students with character tables.
3. To develop an understanding of molecular orbital theory and ligand field theory with respect to symmetry properties.

**UNIT - I**

1. **SYMMETRY ELEMENTS AND OPERATIONS:** Symmetry planes and reflections, inversion centre, proper axes and proper rotations, improper axes and improper rotations. (05)
2. **RELATIONS AMONG SYMMETRY ELEMENTS:** Products of symmetry operations, equivalent symmetry elements and equivalent atoms, general relations among symmetry elements and operations, symmetry point groups, symmetry classification of molecules, virtual labs. (08)

**UNIT - II**

3. **REPRESENTATIONS OF GROUPS:** Important rules about irreducible representations and their characters, relationship between reducible and irreducible representations with examples. Construction of character tables. (08)

**UNIT - III**

4. **MOLECULAR ORBITAL THEORY AND ITS APPLICATIONS:** Symmetry based selection rules for cyclization reactions, dimerization of ethylene, Diels-Alder reactions. (06)
5. **MOLECULAR ORBITAL THEORY FOR INORGANIC COMPOUNDS:** Transformation properties of atomic orbitals, molecular orbitals for sigma bonding in tetrahedral and octahedral molecules. (10)

**UNIT - IV**

6. **LIGAND FIELD THEORY:** Introduction, Electronic structure of free atoms and ions, splitting of levels and terms in a chemical environment, construction of energy level diagram. (08)

**INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

1. Examiner will set total of **NINE** questions comprising **TWO** questions from each unit and **ONE** compulsory question of short answer type covering whole syllabus.
2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks

**BOOKS RECOMMENDED:**

1. F. A. Cotton, **Chemical Applications of Group Theory**, Wiley, 3rd edition, 2004.
2. J.N. Murrell, S.F.A. Kettle, John M Tedder, **Valence Theory**, John Wiley, 1970.
3. R. B. Woodward and R. Hoffmann, **Conservation of Orbital Symmetry**, Academic Press, 1970.
4. B .N. Figgis, **Introduction to Ligand Fields**, John Wiley, 1996.
5. A. Salahuddin Kunju & G. Krishnan, **Group Theory and Its Applications in Chemistry**, PHI Learning Private Limited, New Delhi, 2010.
6. [http://vlab.co.in/ba\\_labs\\_all.php?id=9](http://vlab.co.in/ba_labs_all.php?id=9).

**MSCH-203**  
**SPECTROSCOPY- I**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**3 1 0**

**LEARNING OBJECTIVES:**

1. To educate students about molecular absorption and emission spectroscopy.
2. To understand how the interaction of electromagnetic waves with the matter leads to wonderful results
3. To educate students about atomic absorption and emission spectroscopy.

**UNIT - I**

**1. INTRODUCTION:** Characterization of electromagnetic radiation, the quantization of energy. Regions of the spectrum, representation of the spectrum. Basic elements of practical spectroscopy, Fourier transformation spectroscopy, computer averaging, stimulated emission. (06)

**2. MICROWAVE SPECTROSCOPY:** The rotation of the molecules, rotational spectra, diatomic molecules, polyatomic molecules, techniques and instrumentation, chemical analysis by microwave spectroscopy. Microwave oven. (07)

**UNIT - II**

**3. INFRA-RED AND RAMAN SPECTROSCOPY:** Introduction, the vibrating diatomic molecule, the diatomic vibrating rotator. The vibration-rotation spectrum of carbon monoxide. Breakdown of the Born-Oppenheimer approximation: The interaction of rotations and vibrations. The vibrations of polyatomic molecules, The influence of rotation on the spectra of polyatomic molecules. Analysis by infrared techniques – identity by finger printing and functional groups, techniques and instrumentation. Pure rotational Raman spectra, vibrational Raman spectra. Polarization of light and the Raman effect, Structure Determination from Raman and infrared spectroscopy, techniques and instrumentation, near infrared FT-Raman spectroscopy. Comparison of infrared and Raman spectra. (10)

**UNIT - III**

**4. ELECTRONIC SPECTROSCOPY:** Principles of absorption spectroscopy, the chromophore concept, solvent effects, Woodward-Fieser rules. Applications of electronic spectroscopy. Stereochemical factors. Absorption spectra for charge-transfer complexes, Electronic absorption spectroscopy for chemical analysis. (10)

**UNIT - IV**

**5. ATOMIC ABSORPTION AND EMISSION SPECTROSCOPY:** Introduction, elementary theory, instrumentation. Graphite furnace and cold vapour technique, interferences, background correction methods, Applications of AAS. Emission spectra, flame emission spectroscopy, evaluation methods, plasma emission spectroscopy ICP instrumentation. applications of flame photometry (09)

**6. LUMINESCENCE SPECTROSCOPY:** Principles of luminescence spectroscopy, applications for inorganic & organic compounds. (03)

**INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

1. Examiner will set total of **NINE** questions comprising **TWO** questions from each unit and **ONE** compulsory question of short answer type covering whole syllabus.
2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks.

**BOOKS RECOMMENDED:**

1. C. N. Banewell, **Fundamentals of Molecular Spectroscopy**, 4th Edition, Tata Mc Graw-Hill Publication, 1994.
2. G. N. Barrow, **Introduction to Molecular Spectroscopy**, International Mc.Grw Hill Edition, 4th edition, 1993, UNIT II.
3. D. H. Williams and I. Flemings, **Spectroscopic Methods in Organic Chemistry**, Tata Mc Graw-Hill Publication, 6th edition, 2007.
4. Drago R.S., **Physical Methods in Chemistry**, 3rd ed, Philadelphia, London, W.B. Saunders Company, 1992.
5. W. Kemp, **Organic Spectroscopy**, ELBS Mcmillan, 3rd edition, 1991.

BCET

**MSCH-204**  
**QUANTUM CHEMISTRY**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**3 1 0**

**LEARNING OBJECTIVES:**

1. To learn basic mathematical concepts in quantum chemistry.
2. To understand valence-bond and molecular orbital approaches.
3. To understand and apply perturbation theory.

**UNIT - I**

**1. PREPARATION/REVISION OF BASIC MATHEMATICAL CONCEPTS:** Vectors, dot, cross and triple products etc, gradient, divergence and curl. Matrices – addition, multiplication, adjoint and transpose, special matrices (symmetric, skew-symmetric, hermitian, skew-hermitian, unit, diagonal, unitary etc.). Linear equations, eigen value problem, diagonalization, determinants. Calculus and elementary differential equations - all examples be taken from chemistry. Classical mechanics: Introduction, Lagrange's and Hamilton's equations of motion in classical mechanics, configuration space and phase space. Hermitian operators and their properties. Commutation relations. Postulates of quantum mechanics. Uncertainty principle. Schrodinger equation and its interpretation. (11)

**UNIT - II**

**2. LINEAR HARMONIC OSCILLATOR:** Linear harmonic oscillator and its solution in terms of ladder operators (factorization method). Selection rules, expectation values, virial theorem. Hydrogen atom and its complete solution (including solution of the radial equation using factorization method). Spherical harmonics as wave functions of a rigid rotor. Total wave function of the hydrogen like atoms, shapes of atomic orbitals, Radial distribution function. Virial theorem. Angular momentum, spin coupling of angular momenta; spin-orbit coupling. Term symbols from electronic configuration. (12)

**UNIT - III**

**3. APPROXIMATE METHODS:** Time-Independent (non-degenerate, degenerate states) perturbation theory. Applications of time-dependent perturbation theory. The variation method. LCAO-MO approximation. Comparison of perturbation and variation method. Hartree-Fock equations. configuration interaction. Applications to the electronic structure of many electron atoms, screening, Slater orbitals, Gaussian orbital. (11 )

**UNIT - IV**

**4. THE BORN-OPPENHEIMER APPROXIMATION:** Valence-bond and molecular orbital approaches, their comparison and equivalence limit. Electronic structure of an atomic and polyatomic molecules- an introductory treatment. General molecular orbital theory. The pi-electron approximation. Huckel theory of conjugated systems. Applications to ethylene, butadiene and benzene. (11)

**INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

1. Examiner will set total of **NINE** questions comprising **TWO** questions from each unit and **ONE** compulsory question of short answer type covering whole syllabus.
2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks.



- BOOKS RECOMMENDED:**
1. Atkins P.W. and Friedman R.S., **Molecular Quantum Mechanics**, 4th edition, Oxford University Press, 2005.
  2. McQuarrie D., **Quantum Chemistry**, 2nd edition, University Science Books, 2007.
  3. Levine I.N., **Quantum Chemistry**, 6th edition, Pubs: Prentice Hall, 2009.
  4. Kreyszig E., **Advanced Engineering Mathematics**, 10th edition, John Wiley, 2012.
  5. Ayres F. Jr., **Theory and Problems of Matrices, Schaum's Outline series**, McGraw Hill, New Delhi, part 2, 1974.
  6. Spiegel M.R., **Vector Analysis, Schaum's Outline Series**, McGraw Hill, New Delhi, 1968.
  7. Ayres F., Jr. and Mendelson E., **Schaum's Outline of Theory and Problems of Differential and Integral Calculus**, McGraw hill, New Delhi, 3rd edition, 1990.
  8. Pilar F.L., **Elementary Quantum Chemistry**, 2nd editilon, McGraw Hill, New York, 1990.
  9. March N.H., **Self-Consistent Fields in Atoms**, Pubs: Pergamon Oxford Press, 1975.
  10. Chandra A.K., **Introductory Quantum Chemistry**, Pubs: Tata-McGraw Hill, 4th edition, 2004.
  11. Pople J.A. and Beveridge D.L., **Approximate Molecular-Orbital Theory**, Pubs: McGraw Hill, New York, 1970.
  12. Lowe J.P., Peterson, K, **Quantum Chemistry**, 3rd edition, Academic Press, 2005.

BCET

**MSCH-205**  
**PHYSICAL CHEMISTRY LAB**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**0 0 4**

- (1) Determine the specific rotation of an optically active compound.
- (2) Study the kinetics of inversion of cane sugar by polarimetry.
- (3) Estimate the strength of the strong acid and the weak acid in a mixture by conductometric titration.
- (4) Determine the rate constant of saponification of methyl acetate conductometrically at room temperature.
- (5) Determine the ionization constant ( $K_a$ ) of a weak acid by conductometric method at room temperature and find the equivalent conductance at infinite dilution ( $\Lambda_0$ ) of a weak acid by graphical extrapolation (Verification of Ostwald's dilution law).
- (6) Potentiometrically estimate the strength of Mohr's salt with the help of a standard potassium dichromate solution. Find the  $E_0$ ,  $Fe^{3+} / Fe^{2+}$  using graphical methods.
- (7) Potentiometrically estimate the strength of  $AgNO_3$  solution with a standard  $KCl$  solution. Determine the solubility product ( $K_{sp}$ ) of  $AgCl$  at room temperature.
- (8) Estimate the strength of a weak acid (monobasic/dibasic) pH-metrically. Find  $pK_a$  of this acid at room temperature using a graphical procedure.
- (9) Study the kinetics of the reaction ( $KI + K_2S_2O_8$ ) by colorimetric method and determine the rate constant of the reaction at room temperature.
- (10) Test the validity of Lambert-Beer's law for  $KMnO_4$  solution. Construct similarly the calibration curve for  $K_2Cr_2O_7$  solution and hence determine the concentration of an unknown  $K_2Cr_2O_7$  solution.
- (11) Study the kinetics of iodination of acetone in presence of acid. Hence find out the order with respect to iodine/acetone/acid.
- (12) Determine the critical solution temperature of phenol-water system.
- (13) Determine the solubility product ( $K_{sp}$ ) of  $PbI_2$  and verification of Debye-Hückel limiting law.
- (14) Determination of  $E_0$  of quinhydrone electrode.

**BOOKS RECOMMENDED:**

1. Berry, Rice and Ross, **Physical Chemistry (Topics in Physical Chemistry)**, 2nd edition, Oxford University Press, 2000.
2. Moore, **Physical Chemistry**, 5th edition, prentice hall, 1999. 3. Atkins, **Physical Chemistry**, 9th edition, W.H. Freeman & Co., 2010.
4. Levine, **Physical Chemistry**, 6th edition, McGraw-Hill, 2002.
5. K.J. Laidler, **Chemical Kinetics**, 3rd edition, Pearson Education India, 1987.
6. Zemansky and Dittman, **Kinetics and Mechanism**;
7. Zemansky and Dittman, **Heat and Thermodynamics**, 7th edition, McGrawHill, 2006.
8. Saha and Srivastava, **A Treatise on Heat**, 3rd edition, The Indian Press, 1950.
9. Glasstone, **An Introduction to Electrochemistry**, Affiliated East West Press Private, Limited, 1974.
10. Bockris and Reddy, **Modern Electrochemistry 2A & 2B**, Springer, 2000.

**MSCH-206**  
**ORGANIC CHEMISTRY LAB-II**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**0 0 4**

**1. Beckman Rearrangement**

- I. Benzene-Benzophenone Benzophenone Oxime Benzanilide
- II. Benzene Acetophenone Acetophenone Oxime-Acetanilide.
- III. Cyclohexanone Oxime-Caprolactam.

**2. Benzilic acid Rearrangement**

- I. Benzoin-Benzil-Benzilic-acid
- II. Benzoin-Benzil-Benzil monohydrazone

**3. Fischer Indole Synthesis**

- I. N-Arylmalenilic acid N-aryl maleimide
- II. 1, 2, 3, 4- Tetrahydrocarbazole
- III. 2-Phenylindole from Phenylhydrazone

**BOOKS RECOMMENDED:**

1. **Vogel's Text Book of Practical Organic Chemistry**, 5th edition, Prentice Hall, 1996.
2. Julius B. Cohen, **Practical Organic Chemistry**, 1910.

# BCET

## **Third Semester**

**MSCH-301**  
**INORGANIC CHEMISTRY – II**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**3 1 0**

**LEARNING OBJECTIVES:**

1. To fully understand the chemistry of transition and inner transition elements.
2. To acquaint with organometallic chemistry.
3. To know the structures of ionic solids.
4. To know the advancement of inorganic chemistry in medicine and inorganic compounds in material science.

**UNIT - I**

**1. SURVEY OF TRANSITION METAL CHEMISTRY:** Electronic configuration, general characteristics, oxidation states, pi-acid ligands, metal complexes, metal-metal bond, quadruple bonds. Transition metal catalyzed reactions: Oxidative addition, Elimination reactions and migration reactions. Mechanism of inorganic reactions: Inner sphere, outer sphere, trans effect.

**UNIT - II**

**2. COORDINATION CHEMISTRY:** Coordination number and structures of coordination complexes. Theory of bonding- crystal field and molecule orbital theory. JT distortion, electronic spectra of coordination compounds. Tanabe-Sugano diagrams, stereochemistry of non-rigid and fluxional molecules. Thermodynamic aspects of coordination complexes: Irving William Series. Kinetic aspects: reactions and aquation rates, electron transfer reactions. Reaction mechanisms of inorganic reactions. Redox reactions.

**3. CHEMISTRY OF INNER TRANSITION ELEMENTS:** Electronic configuration, oxidation states, coordination numbers and stereochemistry, Magnetism and spectra, complexes and organometallic chemistry of lanthanides and actinides.

**UNIT - III**

**4. ORGANOMETALLIC CHEMISTRY:** Structure, bonding and reactivity studies of metal carbonyls, nitrosyls, dinitrogen complexes, metal alkyls, carbenes, carbenes and carbides. Metallocenes and related chemistry. Homogeneous and heterogeneous catalysis. Organometallic complexes with metal-metal bonds.

**UNIT – IV**

**5. INORGANIC COMPOUNDS IN MEDICINE AND MATERIALS:** Metal complexes in organic reactions, cis-platin, gold complexes, technetium complexes, metal nano-particles in heterogeneous catalysis, metal embedded polymers as functional materials, metal complexes in display technologies. Inorganic vapochromic materials, molecule-based magnetic materials. DNA cleavage by transition metal complexes, anti-cancer drugs, therapeutic drugs, metal and non-metals in PET.

**INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

1. Examiner will set total of **NINE** questions comprising **TWO** questions from each unit and **ONE** compulsory question of short answer type covering whole syllabus.
2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks.

**BOOKS RECOMMENDED:**

1. D. F. Shriver and P. W. Atkins, **Inorganic Chemistry**, 4th edition, Oxford University, Oxford, 2006.
2. B. N. Figgis, **Ligand Field Theory**, Wiley Eastern, 1976.
3. F. A. Cotton and G. Wilkinson et al, **Advanced Inorganic Chemistry**, 6th edition, John Wiley & Sons, 2003.
4. J. E. Huheey et al, **Inorganic Chemistry**, 4th edition, Pearson, 2005.
5. B. Douglas et al, **Concepts & Model of Inorganic Chemistry**, John Wiley & Sons, New York, 3rd edition, 1994.
6. N. N. Greenwood, **Chemistry of Elements**, Pergamon Press, 2000.

BCET

**MSCH-302**  
**SPECTROSCOPY-II**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**3 1 0**

**LEARNING OBJECTIVES:**

1. To provide students knowledge of various resonance and ionization techniques.
2. To educate the students about the elucidation of structures based on these techniques.
3. To make them familiar with some advanced NMR techniques.

**UNIT – I**

**1. NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY:**

**<sup>1</sup>H-NMR spectroscopy:** Introduction, chemical shift, shielding and equivalence, nuclear magnetic resonance spectrometer, spin-spin splitting rule, coupling constant, protons on oxygen, nitrogen and sulphur. Quadrupole broadening and decoupling. The effect of solvent on chemical shift, chemical shift reagent, chiral resolving agents. Determining absolute and relative configurations via NMR, nuclear overhauser effect difference spectra.

**<sup>13</sup>C NMR spectroscopy:** Introduction, proton-coupled and decoupled <sup>13</sup>C spectra, spin-spin splitting of carbon-13 signals, NOE, molecular relaxation process, DEPT, equivalent carbons, compounds with aromatic ring, carbon-13 NMR solvents, hetero-coupling, coupling constant, magnetic equivalence, first-order and second order spectra, coupling in heteroaromatic system.

**Advanced NMR techniques:** Pulse Sequences and Field Gradients, DEPT experiment, two dimensional spectroscopic methods, correlation spectrometry, COSY, HETCOR, inverse detection method, NOESY experiment, magnetic resonance imaging. Solving a structural problem using combined 1-D and 2-D techniques. (14)

**UNIT – II**

**2. NUCLEAR QUADRUPLE RESONANCE SPECTROSCOPY:** Introduction, experimental considerations, fundamentals of NQR spectroscopy, origin of EFG. Measurement of energy differences between two spin states, the asymmetry parameter, effects of magnetic field. Interpretation of the spectra, applications of technique to halogen compounds, transition metals. Complications in spectra. (07)

**3. ELECTRON PARAMAGNETIC RESONANCE SPECTROSCOPY:** Introduction, principle, presentation of spectrum, hyperfine splitting in isotropic systems involving more than one nucleus, esr spectrum of benzene radical anion, methyl radical, CH<sub>2</sub>OH, cyclopentadienyl radical, cyclopentatrienyl radical, pyrazine anion with <sup>23</sup>Na and <sup>30</sup>K counter ion, nitrosyl nitroxide. Factors affecting magnitude of g values, zero field splitting and Kramer's degeneracy. Qualitative survey of EPR spectra of first row transition metal ion (d<sub>2</sub>, d<sub>3</sub>, low spin d<sub>5</sub>, d<sub>5</sub>, high spin d<sub>6</sub>, d<sub>7</sub>, d<sub>9</sub> system). (07)

**UNIT – III**

**4. MOSSBAUER SPECTROSCOPY:** Principles of Mossbauer spectroscopy, experimental considerations, the spectrum and its parameters. Simple spin states, higher spin states, chemical shift, quadrupole effects. Effects of a magnetic field, applications of Mossbauer spectroscopy – interpretation of Mossbauer spectra. (08)

**UNIT – IV**

**5. MASS SPECTROMETRY:** Overview of the mass spectrometer, ionization methods, mass analysis, Determination of molecular weight and formulae. Structural analysis and fragmentation patterns, strategic approach. Computerized matching of spectra with spectral libraries. (09)

**INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

1. Examiner will set total unit and **ONE** compulsory question of short answer type covering whole syllabus.
2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks.

**BOOKS RECOMMENDED:**

1. R. M. Silverstein and F. X. Webster, **Spectroscopic Identification of Organic Compounds**, 6th Ed., John Wiley & Sons, New York, 1998.
2. D.L. Pavia, G. M. Lampman, George S. Kriz, James R. Vyvyan, **Introduction to Spectroscopy**, 4th Ed., Brooks India, 2008.
3. C. N. Banewell, **Fundamental of Molecular Spectroscopy**, 4th Edition, Tata Mc Graw-Hill Publication, 1995.
4. G. N. Barrow, **Introduction to Molecular Spectroscopy**, Mc Graw Hill Publications, 1980.
5. D. H. Williams and I. Flemings, **Spectroscopic Methods in Organic Chemistry**, Tata Mc Graw-Hill Publication, 1994.
6. R.S. Drago, **Physical methods in Inorganic Chemistry**, Reinhold Publishing Corporation, 1965.

BCET



**MSCH-303**  
**COMPUTATIONAL SKILLS AND SIMULATIONS IN CHEMISTRY**

External Marks: 100

L T P

Internal marks: 50

3 1 0

Total Marks: 150

**LEARNING OBJECTIVES:**

1. To learn principles of computational chemistry and computer-based molecular design.
2. To familiarize with different software packages, including MOLDEN for general model building, GAMESS Gaussian for quantum chemical calculations, and BOSS for liquid simulations.

**UNIT – I**

**1. OVERVIEW OF THE COURSE:** Promises of computational chemistry, molecular mechanics of bond vibrations. Minimization methods, forces in polyatomic molecules, intermolecular forces, parameterization and testing of force fields, docking. (08)

**2. MONTE CARLO METHOD:** Principles, chemical & biochemical applications. (04)

**UNIT – II**

**3. MO THEORY:** Foundations, semi-empirical MO theory, Ab Initio MO Theory: Basis Sets; Hartree–Fock theory: Principles and applications (10)

**UNIT – III**

**4. TREATMENT OF ELECTRON CORRELATION:** MCSCF, CI methods, Treatment of electron correlation: MP and CC methods. (10)

**UNIT – IV**

**5. SPECTROSCOPY:** Vibrational spectroscopy and gas phase thermodynamics, description of electronically excited states. Description of solvent effects. (07)

**6. DENSITY FUNCTIONAL THEORY (DFT):** principles, applications in materials. Transition states in gas phase reactions. (06)

**INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

1. Examiner will set total of **NINE** questions comprising **TWO** questions from each unit and **ONE** compulsory question of short answer type covering whole syllabus.
2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks.

**BOOKS RECOMMENDED:**

1. Peter Comba, Trevor W. Hambley, **Molecular Modelling of Inorganic Compounds**, John Wiley & Sons, 2009.
2. F. Jensen, **Introduction to Computational Chemistry**, John Wiley & Sons, 1998.
3. Warren J. Hehre, **A Guide to Molecular Mechanics and Quantum Chemical Calculations**, 2003.
4. H. D. Holtje, W. Sippl, D. Rognan, G. Folkers, **Molecular Modeling: Basic Principles and Applications**, Wiley, 2008.
5. Christopher Cramer, **Essentials of Computational Chemistry, Theories & Models**, 2nd edition, Wiley, 2002.

Note: Freely available packages like GAMESS, MOLDEN, AVOGADOOS, MOPAC may be used for computational Lab.

# BCET

## **ELECTIVES**

**MSCH-311**  
**POLYMER CHEMISTRY**  
**ELECTIVE-I**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**3 1 0**

**LEARNING OBJECTIVES:**

1. To understand various terms related to polymers.
2. To learn various types of polymer mechanisms and their kinetics.
3. To learn how to characterize polymer structures.

**UNIT-I**

**1. INTRODUCTION TO POLYMERS:** Polymer terminology-fatigue, tensile strength, impact strength, breaking load, crimp, denier, elongation at break, filament, yarn, filament yarn, porosity, resilience, staple fibre, bursting strength, tex, creep, tenacity. IUPAC nomenclature of vinyl, nonvinyl polymers, copolymers and end groups. Abbreviations for polymers. Introduction to industrial polymers-plastics (commonly used commodity- & engineering plastics, thermoplastic- & thermosetting plastics), fibres (commonly used natural & synthetic fibres), elastomers (commonly used natural & synthetic rubbers), coatings and adhesives. Comparison of properties of various types of polymers. Polymer recycling. (06)

**2. POLYMERIZATION MECHANISMS:** Mechanism of free radical chain polymerization & ionic chain polymerization-initiators, inhibitors & stereochemistry. Mechanism of coordination chain polymerization (Ziegler-Natta, Cossee), polycondensation step polymerization, polyaddition step polymerization & ring opening step polymerization. (06)

**UNIT-II**

**3. KINETICS OF POLYMERIZATION MECHANISMS:** Kinetics of free radical chain polymerization, ionic chain polymerization, catalysed and non catalysed polycondensation polymerization including kinetic chain length, chain transfer reactions. (05)

**4. AVERAGE MOLECULAR WEIGHT OF POLYMERS:** Number average molecular weight – its measurement by osmometry (membrane & vapour phase), end group analysis, mass spectrometry. Weight average molecular weight – its measurement by light scattering method (dissymmetry method & Zimm plot method). Viscosity average molecular weight – its measurement by viscometry. Determination of molecular weight distribution by gel permeation chromatography (size exclusion chromatography). (06)

**UNIT-III**

**5. CHEMICAL STRUCTURE & POLYMER MORPHOLOGY:** Macrostructure of polymers. Geometrical isomerism & optical isomerism, Tacticity, degree of crystallinity, liquid crystallinity, crystallizability, crystallites (bundles), spherulites, polymer single (ideal) crystals. Glass transition temperature- concept of glassy state, viscoelastic state, viscofluid state for amorphous and crystalline substances including polymers. Specific volume change vs temperature curves. (05)

**6. POLYMER PROPERTIES:** Mechanical properties - tensile strength, compressive strength, flexural strength, impact strength, toughness, fatigue, yield point, elongation at break, tensile modulus, relaxation & retardation (creep) phenomena. Thermal stability, flammability & flame resistance, chemical resistance, degradability, electrical conductivity, nonlinear optical properties. Polymer additives to modify mechanical, surface, chemical, aesthetic & processing properties. (06)

#### UNIT-IV

**7. FIBRES REINFORCED POLYMER COMPOSITES:** Introduction to composites. Polymer matrix materials & fibres reinforcement. Types of fibres- glass, metal, graphite, boron, alumina, silicon carbide, aramid, quartz & silica fibres. Advantages & disadvantages of polymer composites. (05)

**8. CHARACTERIZATION TECHNIQUES OF POLYMERS:** Infrared, Raman, NMR, ESR, UV-Vis, fluorescence studies. X-ray scattering, SEM, thermal- DSC, DTA, TMA, TGA studies. (06)

#### INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:

1. Examiner will set total of **NINE** questions comprising **TWO** questions from each unit and **ONE** compulsory question of short answer type covering whole syllabus.
2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks.

#### BOOKS RECOMMENDED:

1. D. Campbell and J.R. White, **Polymer Characterization: physical Techniques**, Chapman and Hall, New York, 1989.
2. Malcolm P. Stevens, **Polymer Chemistry an Introduction**, Oxford University Press, 3rd edn, Indian Edition, reprint, 2011.
3. A.H. Fawcett, **Polymer Spectroscopy**, Wiley, New York, 1996.
4. R.J. Young, **Spectroscopy of Polymers**, Wiley, New York, 1996.
5. M. Lewin, S.M. Atlas, E.M. Pearce, **Flame Retardant Polymeric Materials**, Plenum Press, New York, 1975.
6. E.M. Pearce, Y.P. Khanna, D. Raucher, **Thermal Characterization of Polymeric Materials**, Academic Press, New York, 1981.
7. I.M. Ward, **Mechanical Properties of Polymers**, Wiley Interscience, New York, 1971.
8. Jan M. Gooch, **Encyclopedic Dictionary of Polymers**, Springer, 2007.
9. Anita J. Brandolini, Deborah D. Hills, **NMR Spectra of Polymers & Polymer Additives**, Marcel Dekker, New York, 2000.
10. Fred W. Wilmeyer, **Text book of Polymer Science**, A. Wiley Interscience Publication, 1994.
11. V. R. Gowariker, V. R. Gowariker, N.V. Viswanathan, J. Sreedhar; **Polymer Science**, New Age International, 1986.

**MSCH-312**  
**MEDICINAL CHEMISTRY**  
**ELECTIVE-I**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**3 1 0**

**UNIT-I**

**1. ANTIBACTERIAL AND ANTIVIRAL AGENTS:** History of antibacterial drugs, types, classifications, structural activity relationship, fluoroquinolones. Mechanism of action of antibacterial,  $\beta$ -lactams, bacterial resistance against antibacterial drugs. Target for anti HIV drugs, anti HIV agents, HIV-protease inhibitors, amprenavir, foseprenavir, alazanavir etc., anti-HIV nucleosides: lamivudine, retrovir, videx, hivid, zlarit, viread, carbovir, delavirdine, ziduvudine, etavirenz, calanolide, capravine, nevirapine. DNA polymerase inhibitors: acyclovir, ganciclovir, penciclovir, famciclovir, valaciclovir, valomaciclovir, codofvir

**UNIT-II**

**2. ANTIMALARIALS:** Cinchona alkaloids, 4-aminoquinolines, 8-aminoquinolines, pyrimidines and sulfones, 9-aminoacridines, biguanides, mefloquine, sulfonamides.  
**COMMERCIAL SYNTHETIC ROUTES TO:** Chloroquine, pamaquine, primaquine, proguanil, amodiaquine, mefloquine, pyremethamine, sontoquine.

**UNIT-III**

**3. CNS ACTIVE DRUGS: CNS DEPRESSANTS: HYPNOTICS AND SEDATIVES:** Barbiturates, non-barbiturates, amides and imides, glutethimide, benzodiazepines, aldehydes and derivatives, methaqualone and other miscellaneous agents. **ANTICONVULSANTS:** Barbiturates, hydantoin, oxazolindiones, succinimides, benzodiazepines, thenacemide, glutethimide.  
**CNS-STIMULANTS & PSYCHOACTIVE DRUGS:** Analeptics, purines, psychomotor stimulants, sympathomimetics, monamine oxidase inhibitors, tricyclic antidepressants, miscellaneous psychomotor stimulants. Hallucinogens (**psychodelics, psychomimetics**): Indolethylamines, R-phenylethylamines, butyrophenones and other miscellaneous drugs.  
**COMMERCIAL SYNTHETIC ROUTES TO:** Thioridazine, haloperidol, chlorpromazine, phenytoin, Phenobarital, Carbamazepine valproic acid, methaqualone, nitrazepam, oxazepam, diazepam, chloridazepoxide.

**UNIT-IV**

**4. DIURETICS:** Osmotic agents, acidifying salts. Mercurials, purines and related heterocycles, sulfonamides, benzothiadiazene and related compounds, chlorothiazides and analogs, sulfamoylbenzoic acid and analogs, endocrine antagonists, miscellaneous diuretics.  
**COMMERCIAL SYNTHETIC ROUTES TO:** Furosemide, methalthiazide methylchlorothiazide: Chlorothiazide, triameterene, hydrochlorothiazide, amiloride, chlorthalidone.

**INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

1. Examiner will set total of **NINE** questions comprising **TWO** questions from each unit and **ONE** compulsory question of short answer type covering whole syllabus.
2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks.

**BOOKS RECOMMENDED:**

1. Wilson and Gisvolds Textbook of Organic Medicinal and Pharmaceuticals Chemistry, 8th edition, edited by R.F. DeGeorge, J.B. Lippincott Company, Philadelphia, 1982.

2. Pharmaceutical Chemicals in Perspective. B.G. Reuben and H.A. Wittcoff, John Wiley & Sons, NewYork, 1989.
3. W.O. Foye, T.L. Lamke, D.A. Williams, Principles of Medicinal Chemistry, 5th Edition, Lippencott Williams and Wilkins, 2002.

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**MSCH-304**  
**INORGANIC LAB-II**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**0 0 4**

**LEARNING OBJECTIVES:**

1. To know the significant figures and various errors and to understand the principle of working of balances.
2. To become aware of handling of glass wares used in titrimetry.
3. To know the principles of various types of titrimetric analysis.
4. To learn the theory and importance of analytical chemistry.
5. To know the safe working in the Lab and Lab hygiene.
6. To know the methods of analyzing the chemicals by applying the electroanalytical techniques.

**1. INTRODUCTION TO QUANTITATIVE ANALYSIS:** Introduction – types of quantitative analyses – theory of significant figures – error analysis – principles of chemical balances (double-pan and single-pan) – apparatus used in titrimetric analysis – handling of chemical balances and other apparatus – concept of molecular weight, formula weight, equivalent weight – concentrations of solutions – molarity, formality, normality and weight percentage.

**2. GENERAL PRINCIPLES OF TITRIMETRY:** Principle of titrimetry – primary and secondary standards – preparing standard solutions – standardising the secondary standard solutions – types of titrimetric analyses – principal reactions – concepts of acids, bases, oxidants, reductants – theory of indicators – calculations for strengths of solutions and the amounts of substances in solutions.

**3. LABORATORY HYGIENE AND SAFETY:** Storage and handling of corrosive, flammable, explosive, toxic, carcinogenic and poisonous chemicals. Simple first aid procedures for accidents involving acids, alkalis, bromine, burns and cut by glass. Threshold vapour concentration - safe limits. Waste disposal.

**4. COMPLEXOMETRIC TITRATIONS:** Determination of calcium in the presence of magnesium using EGTA as titrant. Determination of the total hardness (permanent and temporary) of water. Determination of calcium in the presence of barium using CDTA as titrant.

**5. REDOX TITRATION:**

- (a) Determination of chlorate, preparation of 0.1M cerium(IV) sulphate solution.
- (b) Determination of copper, determination of dissolved oxygen.
- (c) Determination of hydrogen sulphide.
- (d) Determination of antimony & arsenic.

**6. ELECTRO ANALYTICAL TECHNIQUES-PH METRIC, CONDUCTOMETRIC AND AMPEROMETRIC TITRATION:** Representative acid-base and redox titrations.

**7. COLORIMETRY AND SPECTROPHOTOMETRY:**

- (a) Determination of max the absorption curve and concentration of a substance.
- (b) Simultaneous spectrophotometric determination (chromium and manganese).
- (c) Spectrophotometric determination of pK value of an indicator.
- (d) Determination of copper(II) with EDTA
- (e) Determination of iron(III) with EDTA.

**8. ATOMIC ABSORPTION SPECTROSCOPY:**

- (a) Determination of cations by AAS
- (b) Determination of magnesium and calcium in tap water
- (c) Determination of trace elements in contaminated soil
- (d) Determination of vanadium in lubricating oil, determination of trace lead in a ferrous alloy.

**BOOKS RECOMMENDED:**

1. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, **Vogel's Textbook of Quantitative Analysis**, 6th Ed., Pearson Education, 2000, 3rd reprint.
2. R. Gopalan, P.S. Subramaniam and K. Rengarajan, **Elements of Analytical Chemistry**, 3rd edition, Sultan Chand and Sons, New Delhi, 2003.

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**MSCH-305**  
**COMPUTATIONAL SKILLS AND SIMULATIONS IN CHEMISTRY LAB**

External Marks: 100

Internal marks: 50

Total Marks: 150

L T P

0 0 4

**LEARNING OBJECTIVES:**

To learn a variety of commonly used techniques, such as geometry optimization, location of transition states, conformational analysis, practise on minimization algorithms.

1. Develop force fields and make conformational analysis of small and large molecules.
2. Optimize geometries of some molecules or complexes using Monte Carlo methods.
3. Use semi-empirical methods for optimization of some small or large molecules.
4. Describe electronic structures of molecules by using Hartree - Fock theory.
5. Practise on quantum mechanical harmonic oscillator.
6. Make some comparisons between experimental and calculated molecular vibrations.
7. Prediction of optical spectra after optimizing geometries of transition metal complexes and some porphyrins.

**BOOKS RECOMMENDED:**

1. Peter Comba, Trevor W. Hambley, **Molecular Modelling of Inorganic Compounds**, John Wiley & sons, 2009.
2. F. Jensen, **Introduction to Computational Chemistry**, 2nd edition, Wiley, 2006.
3. Warren J. Hehre, **A Guide to Molecular Mechanics and Quantum Chemical Calculations**, Wavefunction, 2003.
4. H. D. Holtje, W. Sippl, D. Rognan, G. Folkers, **Molecular Modeling: Basic Principles and Applications**, Wiley, 2008.
5. Christopher Cramer, **Essentials of Computational Chemistry**, 2nd edition, Wiley, 2004.

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## **Fourth Semester**

**MSCH-402**  
**ENVIRONMENTAL CHEMISTRY**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**3 1 0**

**LEARNING OBJECTIVES:**

1. To understand how to analyse various constituents of water.
2. To have detailed study of air pollutants.
3. To have knowledge of toxicology of various organic compounds.

**UNIT - I**

Commonly used terms, environmental segments, natural cycles of environment, environmental chemistry of water, water pollution, water treatment operations, advanced waste water treatment.

**UNIT - II**

Analysis of major constituents in water, analysis of common ions at low concentration in water, analysis of trace pollutants in water.

**UNIT - III**

The atmosphere and atmospheric chemistry, air pollutants, organic air pollutants, atmospheric analysis of gases, atmospheric analysis of particulates, soil formation, soil properties, analysis of soil sediments and biological specifications.

**UNIT - IV**

Toxicological chemistry, toxicology of some organic compounds, reactions and rate of hazardous wastes, hazardous waste reduction and minimization and physical methods of treatment of hazardous waste, chemical methods of treatment of hazardous waste.

**INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

1. Examiner will set total of **NINE** questions comprising **TWO** questions from each unit and **ONE** compulsory question of short answer type covering whole syllabus.
2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks.

**BOOKS RECOMMENDED:**

1. De., A.K., **Environmental Chemistry**, 5th Ed., New Age International (P) Limited, New Delhi, 2003.
2. Fifield F.W. and P.J. Hains, **Environmental Analytical Chemistry**, Blackie Academic and professional, Glasgow, UK, 1995.
3. Gary, W. Vanloon. Stephen J. Duffy, **Environmental Chemistry, A global Prospective**, Oxford University Press, 2010.
4. John P. Hager, Barry J Hansen, John F. Pusateri, William P. Imrie, V. Ramachandran, **Extraction and Processing for Treatment and Minimization of Waste, the Mineral, Metal and Material Society**, Pennsylvania, 1994.
5. Rao. C.S., **Environmental Pollution Control Engineering**, New Age International, New Delhi, 2007.

**MSCH-403**  
**ANALYTICAL, MICROSCOPIC AND DIFFRACTION METHODS OF ANALYSIS**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**3 1 0**

**LEARNING OBJECTIVES:**

1. To learn the theory and importance of analytical chemistry.
2. To acquire knowledge about various methods of quantitative estimations.
3. To know the methods of analyzing the chemicals applying the electroanalytical and thermogravimetric instruments.
4. To know the methods of separating the mixture of compounds by chromatographic techniques.
5. To get familiar with various microscopic and diffraction methods of analysis.

**UNIT - I**

- 1. INTRODUCTION TO ANALYTICAL CHEMISTRY:** Types of analytical methods: Importance of analytical methods in qualitative and quantitative analysis: chemical and instrumental methods- advantages and limitations of chemical and instrumental methods. Data handling: Introduction, sensitivity and detection limit, noise and sources, Uncertainties, errors, calibrations, mean, standard deviations. Least square fit, computer aided analysis.
- 2. THERMOANALYTICAL TECHNIQUES:** Principle of thermo gravimetry, differential thermal analysis, differential scanning calorimetry - instrumentation for TGA, DTA and DSC-characteristics of TGA and DTA curves - factors affecting TGA and DTA curves. Applications of thermal analysis.

**UNIT - II**

- 3. ELECTROCHEMICAL TECHNIQUES:** Basic principle, instrumentation and applications of cyclic voltammetry and coulometry, potentiometry, voltammetry, polarography.
- 4. HIGH PERFORMANCE LIQUID CHROMATOGRAPHY:** Principle, instrumentation, supports in HPLC. Applications of HPLC systems, supercritical fluid chromatography(SFC). Recent developments in SFC and applications.

**UNIT - III**

- 5. MICROSCOPY TECHNIQUES:** Basic principle, instrumentation and applications of electron microscopy - SEM, TEM, scanning probe microscopy – AFM.
- 6. X- RAY DIFFRACTION:** Crystal shapes and point groups, reciprocal lattices, unit cells, Miller indices, Bragg's law in reciprocal space, Diffraction pattern assignments, dimensions and contents of the unit cell, X- ray intensities and atomic positions, Fourier synthesis

**UNIT - IV**

- 7. NEUTRON DIFFRACTION:** Elementary theory of neutron diffraction, study of hydrogen bonds, hydrates and other hydrogen containing compounds, magnetism, limitations.
- 8. ELECTRON DIFFRACTION:** Scattering of electrons by gases, visual method, sector method structure of some molecules studies by electron diffraction, limitation of electron diffraction.

**INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

1. Examiner will set total of **NINE** questions comprising **TWO** questions from each unit and **ONE** compulsory question of short answer type covering whole syllabus.
2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks.

**BOOKS RECOMMENDED:**

1. Douglas A. Skoog and Donald M. West, F.J. Holler, **Fundamentals of Analytical Chemistry**, 8<sup>th</sup> edition, Harcourt College Publishers, 2004.
2. J. Mendham, R. C. Denney, J.D. Barnes, M. Thomas, **Vogel's Text Book of Quantitative Chemical Analysis**, 6<sup>th</sup> edition, Pearson Education, 2006.
3. B.K. Sharma, **Instrumental Methods of Chemical Analysis**, Goel Publishing House, Merrut, 1997.
4. R. Gopalan, P.S. Subramaniam and K. Rengarajan, **Elements of Analytical Chemistry**, 3<sup>rd</sup> edition, Sultan Chand and Sons, 2003.
5. S. Usharani, **Analytical Chemistry**, Macmillan Publishers India, 2000.
6. G. H. Stout and L. H. Jensen, **X-ray Structure Determination- A Practical Guide**, 2<sup>nd</sup> edition, Wiley New York, 1989.
7. P.J. Wheatley, **Determination of Molecular Structure**, Oxford, 1968.
8. D. F. Shriver and P. W. Atkins, **Inorganic Chemistry**, , 4<sup>th</sup> edition, Oxford, 2006.
9. A. Braithwaite and F.J. Smith, **Chromatographic Methods**, 5<sup>th</sup> edn., Blackie Academic and Professional, London, 1996.
10. Skoog, Holder, Nieman, **Principles of Instrumental Analysis**, Fifth edition Thomson Books, 1998.

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## **ELECTIVES**

**MSCH-411**  
**NANOCHEMISTRY**  
**ELECTIVE-II**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**3 1 0**

**LEARNING OBJECTIVES:**

1. To understand the concept of self assembly and its applications to various nano structures.
2. To understand synthesis of nano materials.
3. To learn characterization of nano materials.

**UNIT-I**

- 1. INTRODUCTION:** Introduction to nanochemistry and nanotechnology, definition & classification of nanomaterials. Properties & applications of nanomaterials.
- 2. SELF ASSEMBLY AND NANOSTRUCTURES:** Types of self assemblies, self assembling materials. Use of self assembly in nano rod devices, nano wires, nano tubes, molecular logic gates, molecular storage devices, DNA, fullerenes, nano gas sensors.

**UNIT-II**

- 3. NANO MATERIAL SYNTHESIS:** Top down and bottom up approach, synthesis: Vapour phase synthesis by chemical routes; Nucleation & growth from solutions, stabilization against agglomeration. Processing of nano materials; Nano structured sol gel materials. Consolidation of nano crystalline materials by compaction and sintering, nanolithography.

**UNIT-III**

- 4. CHARACTERIZATION TECHNIQUES:** Characterization of nano structured materials – by scattering techniques, proximal microscopy (AFM & STM).

**UNIT-IV**

- 5. SCOPE & OPPORTUNITIES:** Bionano composites, biometrics, nano technology enabled sensors, Microelectronics, drug delivery, bionano information.

**INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

1. Examiner will set total of **NINE** questions comprising **TWO** questions from each unit and **ONE** compulsory question of short answer type covering whole syllabus.
2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks.

**BOOKS RECOMMENDED:**

1. C.P. Poole & F.J. Owens, **Introduction to Nanotechnology**, Wiley, 2003.
2. M. Ratner & D. Ratner, **Nanotechnology**, Prentice Hall, 2003.
3. M. Wilson, K. Kannagara, G. Smith, M. Simmons & B. Raguse, **Nanotechnology**, CRC Press Boca Raton, 2002.
4. A. Ozin Geoffrey & C. Andre, **Nanochemistry, A Chemical Approach to Nanomaterials**, Arsenault Royal Society of Chemists, 2005.
5. E. Foster Lynn, **Nanotechnology, Science Innovation & Opportunity**, Pearson Education, 2007.

**MSCH-412**  
**PHOTOCHEMISTRY**  
**ELECTIVE-II**

**External Marks: 100**  
**Internal marks: 50**  
**Total Marks: 150**

**L T P**  
**3 1 0**

**LEARNING OBJECTIVES:**

1. To understand various types of photo reactions.
2. To learn photochemical reactions in inorganic chemistry.
3. To study kinetics of photochemical reactions.

**UNIT - I**

**1. ORGANIC PHOTOCHEMISTRY:** Organic photochemistry: Photochemical reactions, fate of excited molecules, Jablonski diagram, Norish type I and Norish II reactions, photoreduction (of ketones), photoaddition reactions, Paterno-Buchi reactions, di-pi methane rearrangement, photo oxidation (formation of peroxy compounds), photo-isomerization (cis-trans isomerisation), photo-addition of olefin and amines to aromatic compounds, photo-rearrangements; Photo-Fries rearrangement. (11)

**UNIT - II**

**2. INORGANIC PHOTOCHEMISTRY:** Photo-substitution, -redox, -isomerization, and -rearrangement reactions in inorganic complexes, photovoltaic and photo-galvanic cells- photo-electrochemical cells- photo assisted electrolysis of water, application of metal complexes in solar energy conversions. (11)

**UNIT - III**

**3. PHYSICAL PHOTOCHEMISTRY:** Absorption and emission of radiation-Frank Condon principle, spin allowed and spin forbidden transitions. Radiative processes- fluorescence and phosphorescence (factors affecting fluorescence and phosphorescence and theory) prompt and delayed fluorescence and quenching of fluorescence- static and dynamic quenching-Stern Volmer equation, Non-radiative processes, theory of radiationless transition, internal conversion and intersystem crossing. (11)

**UNIT - IV**

**4. TECHNIQUE AND APPLICATIONS OF PHOTO-CHEMISTRY:** Techniques and applications of photochemistry – quantum yields- experimental determination of quantum yield, actinometry- chemical actinometry, steady state treatment of quantum yield- reasons for low and high quantum yield- life time measurement- relative and non-relative lifetime measurement- kinetics of photochemical reactions, photosensitized reactions. (12)

**INSTRUCTIONS FOR PAPER SETTERS AND CANDIDATES:**

1. Examiner will set total of **NINE** questions comprising **TWO** questions from each unit and **ONE** compulsory question of short answer type covering whole syllabus.
2. The students are required to attempt **FIVE** questions in all, **ONE** question from each unit and the compulsory question.
3. All questions carry equal marks.

**BOOKS RECOMMENDED:**

1. **Principles of Molecular Photochemistry: An Introduction.**
2. Nicholas J. Turro, **Modern Molecular Photochemistry.**