

*Academic Session: 2020-21*

# FACULTY OF SCIENCES

## SYLLABUS

### FOR

## M.Sc. Chemistry

(Semester I-IV)

Session: 2020-21



## KHALSA COLLEGE AMRITSAR

*(An Autonomous College)*

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**Defaulters will be prosecuted.**

**(ii) Subject to change in the syllabi at any time.**

**Please visit the College website time to time.**

## Scheme of Courses

**Eligibility:-**The candidate having passed B.Sc. degree (10+2+3 system of education) with Chemistry as one of the elective subject with at least 50% marks from Guru Nanak Dev University or any other examination recognized equivalent there to by the University.

<b>Semester-I</b>			
<b>Subject Code</b>	<b>Subject</b>	<b>Max. Marks</b>	<b>Hrs</b>
Course-CH401/MHCH401	Inorganic Chemistry-I: ( <i>Ligand Field and Group Theory</i> )	50	45
Course-CH402	Organic Synthesis-I ( <i>Reaction Mechanism-Substitution reactions</i> )	50	45
Course-CH403/MHCH403	Physical Chemistry-I: <i>Thermodynamics</i>	50	45
Course-CH404/MHCH404	Spectroscopy A: <i>Techniques for Structure Elucidation of Organic Compounds</i>	75	60
Course-CH405/MHCH405	Computer for Chemists – Theory	25	30
Course-CH406/MHCH406	Computer for Chemists – Practical	25	45
Course-CH407/MHCH407	Inorganic Chemistry Lab-I ( <i>Quantitative Analysis</i> )	100	60
Course-CH408	Organic Chemistry Lab- I	100	60
<b>TOTAL</b>		<b>475</b>	<b>370</b>
<b>Semester-II</b>			
<b>Subject Code</b>	<b>Subject</b>	<b>Max. Marks</b>	<b>Hrs</b>
Course-CH409	Inorganic Chemistry-II: ( <i>Reaction Mechanism, Organometallics and Catalysis</i> )	50	45
Course-CH410/ MHCH 410	Organic Synthesis-II ( <i>Reaction Mechanism-Addition, Elimination and Rearrangements</i> )	50	45
Course-CH411/ MHCH411	Physical Chemistry-II: <i>Quantum Chemistry</i>	50	45
Course-CH412/ MHCH412	Spectroscopy B: <i>Techniques for Structure Elucidation of Inorganic Compounds</i>	75	60
Course-CH413/ MHCH413	Organic Synthesis-III( <i>Supramolecular, Reactive Intermediates and Disconnections</i> )	50	45
Course-CH414(a)/ MHCH414(a)	Mathematics for Chemists(Medical Students)	25	30
Course- CH414(b)/MHCH414(b)	Biology for Chemists(Non Medical Students)		
Course-CH415/MHCH415	Physical Chemistry Lab-I	100	60
Course-CH416/MHCH416	Inorganic Chemistry Lab- II	100	60
<b>TOTAL</b>		<b>500</b>	<b>385</b>

<b>Semester-III</b>			
Subject Code	Subject	Max. Marks	Hrs
Course-CH417/MHCH417	Inorganic Chemistry-III: ( <i>Bioinorganic and Metal Clusters</i> )	50	45
Course-CH418/MHCH418	Organic Synthesis-IV ( <i>Natural Products</i> )	50	45
Course-CH419	Physical Chemistry-III ( <i>Electrochemistry and Chemical Dynamics</i> )	75	60
Course-CH420/MHCH420	Organic Synthesis-V ( <i>Pericyclic &amp; Photochemistry</i> )	50	45
Course-CH421/MHCH421	Physical Chemistry-IV ( <i>Analytical Techniques</i> )	50	45
Course-CH422	Organic Chemistry Lab- II	100	60
Course-CH423	Physical Chemistry Lab-II	100	60
<b>TOTAL</b>		<b>475</b>	<b>360</b>
<b>Allocation of Project and Literature Survey</b>			

<b>Semester-IV</b>			
Subject Code	Subject	Max. Marks	Hrs
Course-CH424/MHCH423	Inorganic Chemistry-IV: ( <i>Advanced Inorganic Chemistry</i> )	75	60
Course-CH425/MHCH424	Organic Synthesis-VI ( <i>Asymmetric synthesis, Green Chemistry and Heterocyclic Chemistry</i> )	75	60
Course-CH426/MHCH425	Physical Chemistry-V ( <i>Surface and Polymer Chemistry</i> )	75	60
<b>TOTAL</b>		<b>225</b>	<b>180</b>
<b>Experimental Project Handling and its Presentation</b>			

**Distribution of Marks**

SNo.	Semester	Total Marks
1	Semester-I	475
2	Semester-II	500
3	Semester-III	475
4	Semester-IV	225
<b>Grand Total</b>		<b>1675</b>

**Important Note: M. Sc. (Chemistry) and M. Sc.(Hons.) Chemistry have some common subjects.**

**The subject code of M. Sc. (Chemistry) starts with**

**CH...,**

**The subject codes of M. Sc. (Hons.) Chemistry starts with**

**MHCH...**

# *Semester-I*

*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-I)*  
**CH 401/MHCH 401: Inorganic Chemistry-I**  
*Ligand Field and Group Theory*

45 Hrs.

Time: 4 Hrs/week.

Max. Marks: 37+13 (Internal Assessment)

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of nine short questions carrying 1 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 7 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**1. Group theory and its applications-I**

**11 Hrs**

Symmetry, symmetry elements and operations, Determination of point groups(flow chart), Order and class of point group, Reducible and irreducible representations( $H_2O$  and  $BF_3$ ). Multiplication tables and derivation of character tables for  $C_{2V}$ ,  $C_{3V}$  and cyclic group, Great orthogonality theorem, Mullikens notations.

**UNIT-II**

**2. Group theory and its applications-II**

**11 Hrs**

Crystallographic Symmetry, Sub groups, determination of symmetry of atomic orbitals under different point groups. Hybridisation of atomic orbitals:  $sp$ ,  $sp^2$ ,  $sp^3$ ,  $dsp^2$ ,  $sp^3d$  and  $d^2sp^3$  and group theory, Matric representation of symmetry operations, group theory and CFT. Separation of d-orbitals under the influence of  $T_d$ , square planar,  $O_h$  and trigonalbipyramid symmetry, Vibrational modes in non-linear molecules, representation of vibrational modes in  $H_2O$ ,  $NH_3$  and  $BF_3$ . Group theory and linear molecules.

**UNIT-III**

### **3. Ligand Fields-I**

**11Hrs**

Concept and scope of ligand fields, d and other orbitals, Qualitative determination of ligand field effects, the physical properties affected by LF, Ionic model of coordination compounds, Spin-orbit coupling, free ion in weak CF, Effect of cubic field on S,P,D,F,G,H,I terms.

Heat of ligation and CFSE, Standard electrode potential and CFSE, Cation distribution in lattice, spinels, interionic separation and CFSE and chemical stability.

## **UNIT-IV**

### **4. Ligand Fields-2**

**12Hrs**

Free ion in medium and strong fields. Transition from weak to strong fields, Correlation and Tanabe Sugano diagrams for  $d^2$  to  $d^9$  ( $O_h$  and  $T_d$ ), Elementary MOT, Bonding in octahedral and tetrahedral complexes.

Qualitative calculations of  $10 Dq$ . Electronic spectra of complexes, Selection rules and band widths and factors, Jahn Teller effect. Spectra of  $[M(H_2O)_6]^{+2}$ .

Spectra of spin free and paired complexes, distorted  $O_h$  and  $T_d$  complexes, Spectrochemical and Nephelauxetic series and CT spectra.

#### **Books Recommended:**

- 1) Chemical applications of Group theory by F.A. Cotton.
- 2) Introduction to Ligand fields by B.N. Figgis.
- 3) Group theory by Raman.
- 4) Group theory in Chemistry by Gopinathan and Ramakrishnan.

*M.Sc. Chemistry (Semester-I)*  
**CH 402: Organic Synthesis-I**  
*Reaction Mechanism-Substitution Reactions*

**45 Hrs.**

**Time: 4 Hrs/week.**

**Max. Marks: 37+13 (Internal Assessment)**

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of nine short questions carrying 1 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 7 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**1. Reaction Mechanism: Structure and Reactivity**

**10 Hrs**

Type of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Hard and soft acids and bases.

Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes.

Effect of structure on reactivity- resonance and field effects, steric effect, quantitative treatment.

The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

**UNIT-II**

**2. Stereochemistry :**

**7 Hrs**

Elements of symmetry, chirality, molecules with more than one chiral center. Threo and erythro isomers, methods of resolution, optical purity.

Prochirality – enantiotopic and diastereotopic atoms, groups and faces.

Stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in absence of chiral carbon (Biphenyls, Allenes, Spiranes). Chirality due to helical shape.

**3. Aliphatic Electrophilic Substitutions**

**5 Hrs**

*Bimolecular mechanisms-  $S_E2$  and  $S_{Ei}$ : The  $S_{E1}$  mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity, Hell-Volard-Zelinsky reaction ,*

### UNIT-III

#### 4. Aliphatic Nucleophilic Substitutions

8 Hrs

The  $S_N2$ ,  $S_N1$ , missed  $S_N1$  and  $S_N2$  and SET mechanisms. The neighbouring group mechanism, neighbouring group participation by  $\pi$  and  $\sigma$  bonds, anchimeric assistance.

Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. The  $S_N1$  mechanism,

Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium,

Phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity. Gabriel synthesis

#### 5. Aromatic Nucleophilic Substitution

5 Hrs

The  $S_NAr$ ,  $S_N1$ , benzyne and  $S_{RN}1$  mechanisms, Reactivity-effect of substrate structure, leaving group and attacking nucleophile.

The von Richter, Sommelet-Hauser, and Smiles rearrangements.

### UNIT-IV

#### 6. Aromatic electrophilic substitution

5 Hrs

The arenium ion mechanism, orientation and reactivity in mono substitution and disubstituted aromatics, energy profile diagram, the *ortho/para* ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles.

Diazo coupling, Vilsmeier reaction, Gatterman-Koch reaction, Bechmann reaction, Hoesch reaction.

#### 7. Free Radical Reactions

5 Hrs

Types of free radical reactions, free radical substitution mechanism, 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, autooxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

#### Books Recommended:

1. Stereochemistry - Eliel
2. Advanced Organic Chemistry – Jerry March.
3. Advanced Organic Chemistry, F. A. Carey, R. J. Sundberg, Volume I and II
4. Highlights of Organic Chemistry, W.J. L. Nobel; An Advanced Text Book.
5. Stereochemistry conformation and Mechanism – P. S. Kalsi



*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-I)*  
**CH 403/MHCH 403: Physical Chemistry**  
*Thermodynamics*

45 Hrs.

Time: 4 Hrs/week.

Max. Marks: 37+13 (Internal Assessment)

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of nine short questions carrying 1 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 7 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**1. Classical Thermodynamics-I**

**11Hrs**

Brief resume of concepts of thermodynamics, Helmholtz and Gibb's free energy, chemical potential and entropy. Partial molar properties, partial molar free energy, partial molar volume and partial molar heat content and their significances. Determination of these quantities. Concept of fugacity and determination of fugacity.

**UNIT-II**

**2. Classical Thermodynamics-II**

**11 Hrs**

Non-ideal systems: Excess functions for non-ideal solutions. Activity, activity coefficients, Debye-Huckel theory for activity coefficient of electrolytic solutions, determination of activity and activity coefficients, ionic strength.

**UNIT-III**

**3. Statistical Thermodynamics:**

**13Hrs**

Thermodynamic probability, Most probable distribution, Stirling approximation, Maxwell-Boltzmann distribution law, Entropy and probability, Ensemble averaging, postulates of ensemble averaging. Types of ensemble systems, Lagrange's method of undetermined multipliers.

Partition functions: Translational, rotational, vibrational and electronic partition function, calculation of thermodynamic properties in terms of partition functions. Application of partition functions in the determination of equilibrium constants and heat capacity behavior of solids-chemical equilibria.

Types of statistics: Fermi-Dirac statistics-distribution laws, Bose-Einstein statistics- distribution law and application to helium.

**UNIT-IV**

**4. Non Equilibrium Thermodynamics:**

**10 Hrs**

Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes: heat flow, chemical reactions, transformations of generalized fluxes and forces, non-equilibrium stationary states, phenomenological equations, microscopic reversibility, irreversible thermodynamics for biological systems, coupled reactions.

**Books recommended:**

1. S. Glasstone: Thermodynamics for Chemists
2. P.W. Atkins: Physical Chemistry
3. S.H. Maron & C.F. Prutton: Principles of Physical Chemistry
4. Introduction to the Thermodynamics of Biological Processes by D. Jou & J. E. Lebot.
5. Pitts: Non equilibrium thermodynamics
6. I Prigogine: Introduction to thermodynamics of irreversible processes

*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-I)*

**CH 404/MHCH 404: Spectroscopy-A**

*Techniques for Structure Elucidation of Organic Compounds*

**60 hrs.**

**Time: 6 Hrs/week.**

**Max. Marks: 56+19 (Internal Assessment)**

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of EIGHT questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of eight short questions carrying 1 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 12 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**1. General Features of Spectroscopy:**

**3 Hrs**

Units and conversion factors. Introduction to spectroscopy, Nature of radiation. Energies corresponding to various kinds of radiation, Experimental techniques, intensities of spectral lines, Selection rules and transition moments, Line widths, Broadening.

**2. Nuclear Magnetic Resonance Spectroscopy-I**

**12Hrs**

PMR: Natural abundance of  $^{13}\text{C}$ ,  $^{19}\text{F}$  and  $^{31}\text{P}$  nuclei; The spinning nucleus, effect of external magnetic field, precessional motion and frequency, Energy transitions, Chemical shift and its measurements. Factors influencing chemical shift, anisotropic effect; Integrals of protons, proton exchange, spin-spin coupling- splitting theory, one, two and three bond coupling, virtual, long range and allylic coupling, magnitude of coupling constant; factors affecting the coupling constant, Chemical and magnetic equivalence, First and second order spectra,  $A_2$ , AB, AX,  $AB_2$ ,  $AX_2$ ,  $A_2B_2$  and  $A_2X_2$  spin systems.

**UNIT-II**

**3. Nuclear Magnetic Resonance Spectroscopy-2**

**13 Hrs**

Simplification of complex spectra (solvent effect, field effect, double resonance and lanthanide shift reagents), CW and FT NMR, Relaxation processes, T1 and T2 measurements, Applications of PMR in structural elucidation of simple and complex compounds.  $^{13}\text{C}$ -NMR: Resolution and multiplicity of  $^{13}\text{C}$  NMR,  $^1\text{H}$ -decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; NOE and origin of nuclear overhauser effect. off-resonance, proton decoupling.

Structural applications of  $^{13}\text{C}$ -NMR., pulse sequences, pulse widths, spins and magnetization vectors, DEPT, INEPT.

Introduction to 2D-NMR, COSY, NOESY, HSQC spectra

**UNIT-III**

**3. Mass Spectra:**

**8**

**Hrs** Introduction, methods of ionization EI & CI, Brief description of LD, FAB, SIMS, FD etc., Ion analysis methods (in brief), isotope abundance, Metastable ions, general rules predicting the fragmentation patterns. Nitrogen rule, determination of molecular ion peak, index of H deficiency, fragmentation patterns for aliphatic compounds, amines, aldehydes, Ketons, esters, amides, nitriles, carboxylic acids ethers, aromatic compounds etc.

**4. UV and Visible Spectroscopy of organic molecules:**

**8 Hrs**

Measurement techniques, Beer – Lambert's Law, molar extinction coefficient, oscillator strength and intensity of the electronic transition, Frank Condon Principle, Ground and first excited electronic states of diatomic molecules, relationship of potential energy curves to electronic spectra, Chromophores, auxochromes, blue shift, red shift, hypo and hyperchromic effect,  $n-\sigma^*$ ,  $\pi-\pi^*$ ,  $n-\pi^*$  transitions in organic molecules.

Woodward rules for conjugated dienes and  $\alpha,\beta$ -unsaturated carbonyl groups, extended conjugation and aromatic sterically hindered systems, Quantitative applications.

**UNIT-IV**

**5. Infrared Spectroscopy**

**8 Hrs**

Vibrational Energy Levels, Selection Rules, Force Constant, Fundamental Vibration frequencies, Factors influencing Vibrational Frequencies (Vibrational Coupling, Hydrogen Bonding, electronic effect, Bond Angles, Field Effect). Sampling Techniques, Absorption of Common functional Groups, Interpretation, Finger print Regions.

**Applications in Organic Chemistry**

- (a) Determining purity and quantitative analysis.
- (b) Studying reaction kinetics.
- (c) Determining purity and quantitative analysis.
- (d) Studying hydrogen bonding.
- (e) Studying molecular geometry & conformational analysis.
- (f) Studying reactive species

**6. Solution of Structural Problems by Combined Use of the following Spectroscopic Techniques**

**8Hrs**

- (a) Electronic spectra
- (b) Vibrational spectroscopy
- (c) NMR ( $^1\text{H}$  and  $^{13}\text{C}$ ) spectroscopy
- (d) Mass Spectroscopy

**Books Recommended:**

1. Pavia, Lampman & Kriz, Introduction to Spectroscopy.
2. C.N Banwell "Fundamentals of Molecular Spectroscopy".
3. R. M. Silverstein, G.C. Bassler, T.C. Morrill, "Spectrometric Identification of Organic Compounds.
4. W. Kemp, "Organic Spectroscopy".
5. D.H. Williams, I. Fleming, "Spectroscopic Methods in Organic Chemistry".
6. D.H. Williams, I. Fleming, "Spectroscopic Problems in Organic Chemistry", 1967.
7. R.C. Banks, E.R. Matjeka, G. Mercer, "Introductory Problems in Spectroscopy", 1980.

8. G.M. Barrow "Introduction to Molecular Spectroscopy".

*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-I)*

**Computer for Chemists**

**Theory Code: CH 405/ MHCH 405**

**(Theory 30Hrs + Practical 30Hrs)**

**Max. Marks: 50**

**Theory Marks: 18+7(Internal Assessment) Practical Marks: 18+7(Internal Assessment)**

The paper will consist of 30 Hours of teaching in class room and 15 sessions of 2 hours of practical training on computers. The theory will be of 25 (18+7) marks and practical would be of 25 (18+7) marks. The students would prepare a record of the programs written by them along with the outputs.

**Instructions for paper setters and candidates**

The question paper should consist of three sections.

**Section-A**

It consist of 4 questions and each question carries 1 mark. All questions are compulsory to attempt. Total weightage of this section will be 04 Marks

**Section-B**

It consist of 4 questions and attempt any 2 questions. Each question carries 3.5 marks. Total weightage of this section will be 07 Marks

**Section-C**

It consist of 4 questions and attempt any 2 questions. Each question carries 3.5 marks. Total weightage of this section will be 07 Marks

**1. Computer Programming in C language 30 Hrs**

**Unit-I**

Principles of programming, algorithms and flowcharts.

Elementary programming, a typical C program, printf function.

Introduction of declarations, assignments and variables: concept of an integer, concept of a variable, rules for naming variables, assignment statement, arithmetic operators.

Integer arithmetic expressions, truncation effects, relative priority of arithmetic operators, use of parenthesis, modulus operator.

Floating point numbers, scientific notation, converting integers to floating point and vice versa , coercion and cast operator, type char.

**Unit-II**

Decision making in C, scan f function, relational operators, logical operators, if statement, if else statement, nesting of if statement. The while loop, do while loop, for loop, nesting of for loop.

Type char and ASCII code, character strings and how to print them, octal and hexadecimal notation. User defined functions, returning value from a function, functions with more than one parameters. Arrays, declaring an array, initializing an array, break statement, strings and character arrays, sorting an array, finding maximum and minimum in an array, multidimensional arrays. Input and output.

## **Practical**

### **Practical Code: CH 406/ MHCH 406**

#### **1. Practical based on Microsoft Word and Microsoft Powerpoint**

#### **2. Computer programs in Chemistry**

Development of small computer codes involving simple formulae in chemistry:

1. Calculation of mean, median, mode.
2. Solution of a quadratic equation.
3. Calculation of linear regression.
4. Calculation of curve linear regression.
5. Calculation of Bohr orbit from de Broglie Lambda for electron.
6. Calculation of wave number and frequency from value of wave length.
7. Calculation of van der Waals radii.
8. Radioactive decay.
9. Rate constant of a 1st order reaction, 2nd order reaction.
10. Determination
11. Calculation of lattice energy using Born Lande equation.
12. Addition, multiplication and solution of inverse of 3 X 3 matrix.
13. Calculation of average molecular weight of a polymer containing n1 molecules of molecular weight m1, n2 molecules of molecular weight M2 and so on.
14. Program for calculation of molecular weight of organic compound containing C, H, N, O and S.
15. Calculation of reduced mass of diatomic molecule.
16. Calculate the RMS and most probable velocity of a gas.
17. Calculate the ionic mobility from ionic conductance values.
18. Determine the thermodynamic parameters for isothermal expansion of monoatomic ideal gas.
19. Calculation of value of g- factor from value of J and S.
20. Calculate the bond length and bond angles using crystal structure data.

#### **Recommended Books:**

1. K.V. Raman, Computers in Chemistry, Tata McGraw Hill.
2. Mullish Cooper, The spirit of c, An Introduction to Modern Programming.
3. "Let Us C" by Yashavant Kanetkar
4. Programming ith C by Byron S. Gottfried, Tata McGraw Hill

*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-I)*  
**CH 407/MHCH 407: Inorganic Chemistry Practical-I**  
*Quantitative analysis*

**Max. Marks: 75+25(Internal Assessment)**

**Labs Hrs.: 60**

**I. Oxidation-Reduction Titrations**

1. Standardization with sodium oxalate of  $\text{KMnO}_4$  and determination of  $\text{Ca}^{2+}$  ion.
2. Standardization of ceric sulphate with Mohr's salt and determination of  $\text{Cu}^{2+}$ ,  $\text{NO}_3^-$  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.

**II. Precipitation Titrations**

1.  $\text{AgNO}_3$  standardization by Mohr's method by using adsorption indicator.
2. Volhard's method for  $\text{Cl}^-$  determination.
3. Determination of ammonium / potassium thiocyanate.

**III. Complexometric Titrations**

1. Determination of  $\text{Cu}^{2+}$  and  $\text{Ni}^{2+}$  by using masking reagent by EDTA titration.
2. Determination of  $\text{Ni}^{2+}$  (back titration).
3. Determination of  $\text{Ca}^{2+}$  (by substitution method).

**IV. Gravimetric Analysis**

1. Determination of  $\text{Ba}^{2+}$  as its chromate.
2. Estimation of lead as its lead molybdate.
3. Estimation of chromium (III) as its lead chromate.
4. Estimation of  $\text{Cu}^{2+}$  using Ammonium/ Sodium thiocyanate.

**Book:** Vogel's book on Inorganic Quantitative Analysis.



*M.Sc. Chemistry (Semester-I)*  
**CH408: Organic Chemistry Lab-I**  
*Quantitative analysis and Multistep Synthesis*

**Max. Marks: 75+25 (Internal Assessment)**

**Labs Hrs.: 60**

**1. Quantitative Analysis**

**(a) Extraction of Organic Compounds from Natural Sources**

1. Extraction of Caffeine from tea leaves
2. Isolation of casein from milk (try some typical colour reactions proteins).
3. Isolation of essential oils from Caraway seeds and orange peels – (S) – Carvone and (R) – Limonene

**(b) Quantitative Analysis of Organic Compounds:**

1. Estimation of phenol/aniline using bromate-bromide solution.
2. Estimation of reducing sugar by Fehling solution method.
3. To determine the saponification value of the given fat or oil sample.
4. To determine the iodine number of the given fat or oil sample.

**2. Multistep Organic Synthesis**

1. Synthesis of 2-chloro-4-bromoaniline from aniline (Bromination and chlorination)
3. Photochemical synthesis of benzpinacol and its pinacol rearrangement.
4. Synthesis of o-chlorobenzoic acid from phthalimide. Synthesis of acridone from o-chlorobenzoic acid. (Hofmann bromamide and Sandmeyer's reaction).
4. Synthesis of 2,4-dinitrophenyl hydrazine from chloro benzene. (Electrophilic and nucleophilic substitution reactions on aromatic ring).
5. Synthesis of 2-phenylindole-Fischer Indole Synthesis. Synthesis of 3-nitrobenzoic from benzoic acid
6. Cannizaro's reaction of 4-chlorobenzaldehyde..

**Book Recommended:**

1. Vogel's Textbook of Practical Organic Chemistry

# *Semester-II*

*M.Sc. Chemistry (Semester-II)*  
**CH409: Inorganic Chemistry-II**  
*Reaction Mechanism, Organometallics and Catalysis*

45 Hrs.

Time: 4 Hrs/week.

Max. Marks: 37+13 (Internal Assessment)

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of nine short questions carrying 1 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 7 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**12Hrs**

Energy, polarity and reactivity of M-C bond, stability and lability of main group organometallics and their preparation.

Li organometallics: Structure, bonding and reactions. Carbolithian. Organometallics of group 2 and 12:

Organometallics of Be and Mg: Preparation, mechanism of formation and constitution, Grignard reagent in solution and reactions.

Organometallics of Zn, Cd, Hg: Preparation, structure and properties. Technical applications of tris(alkyl)aluminium compounds.

Organometallics of transition elements: EAN rule and MOT relationship in  $O_h$  sigma and  $O_h$  sigma and  $\pi$  bonding. The particular case of  $d^8$  and  $d^{10}$  complexes. Sigma and  $\pi$  donor/acceptor ligands.

**UNIT-II**

**11Hrs**

Olefin complexes: Preparation, structure and bonding. Alkyne and allyl complexes: Preparation, structure and reactions. Complexes of cyclic  $\pi$  parameter  $C_nH_n$ ; Sandwich complexes, Half sandwich complexes, Multidecker sandwich complexes, Tilted sandwich structure, complexes with more than two  $C_nH_n$  ligand.  $C_4H_4$  and  $C_5H_5^-$

Organometallics: Preparation, structure, reactions and bonding. MOT for ferrocene and bis(benzene)chromium(0) : preparation and reactions. Cycloheptatrienyl and COT complexes: preparation and structure and bonding.

Catalytic reactions and 16/18 electron rule, alkenemetathesis, Chauvin mechanism, Olefin polymerization, Ziegler-Natta polymerization, Cossemechanism, hydrogenation of alkenes,

Wilkinson's catalyst, Fischer-Tropsch reactions, water gas shift reactions, Monsanto acetic acid process, hydrocyanation, Reppe carbonylation, hydroformylation of unsaturated compounds.

### UNIT-III

12Hrs

Reductive carbonylation of alcohols and other compounds, carbonylation reactions: methanol and methyl acetate, adipic ester and other compounds, synthesis and carbonylation reactions, decarbonylation reaction, catalytic addition of molecules to carbon-carbon multiple bonds, homogeneous hydrogenation, hydrocyanation and hydrosilation of unsaturated compounds, polymerization. Oligomerisation and metathesis of alkene and alkynes. Cluster compounds in catalysis, supported homogeneous and phase transfer catalysis, oxidation reactions, oxidative carbonylation. Pd catalysed oxidation of ethylene, acrylonitrile synthesis, oxygen transfer from peroxo and oxo species and NO<sub>2</sub> groups.

Ligand replacement reaction, Labile and Inert complexes and CFT, water exchange rates, formation of complexes from aqueous ions, Anation, Aquation and acid-base hydrolysis, Mechanism of acid hydrolysis when inert ligand is a  $\pi$  donor/acceptor and cis to leaving group, attack on ligands.

Substitution in square planar complexes, factors, trans effect, its theories and applications, Kurnakov test.

### UNIT-IV

10Hrs

Metal carbonyl reactions, reactions of binuclear carbonyls, associative reactions, species with 17 electrons, electron transfer processes, orbital occupation effects on substitution reactions of octahedral complexes. Synthesis of coordination compounds by substitutional reactions, synthetic chemistry of some cobalt and platinum complexes. Marcus theory and applications, electron transfer reactions, doubly bridged inner sphere, electron transfer, other electron transfer, two electron transfer reactions, complimentary and non-complimentary reactions. Ligand exchange *via* electron exchange, Stereochemical non-rigidity of complexes and organometallics and NMR, trigonal and trigonal bipyramidal molecules, system with coordination number 6 and more. Isomerisation and racemisation of tris chelates complexes and mechanism. Metal carbonyl scrambling, Rotation within coordination sphere.

#### Recommended Books:

- 1) F.A. Cotton and I.G. Wilkinson, Advanced Inorganic Chemistry, 5<sup>th</sup> ed. New YORK 1988.
- 2) Organometallics by Salzer.

*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-II)*

**CH 410/MHCH 410: Organic Synthesis-II**

*Reaction Mechanism- Addition, Elimination and Rearrangement Reactions*

**45 Hrs.**

**Time: 4 Hrs/week.**

**Max. Marks: 37+13 (Internal Assessment)**

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of nine short questions carrying 1 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 7 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**1. Addition to Carbon-carbon and Carbon-Hetero Multiple Bonds-I**

**12Hrs**

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropaning. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation. Addition of Grignard reagents, organozinc, organolithium and Gilman reagents to carbonyl and unsaturated carbonyl compounds. Use of other organometallic reagents in addition reactions. Wittig reaction,

**UNIT-II**

**2. Addition to Carbon-carbon and Carbon-Hetero Multiple Bonds-II**

**3Hrs**

Mechanism of condensation reactions involving enolates – Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions.

Hydrolysis of esters and amides, ammonolysis of esters.

**3. Rearrangements and Coupling Reactions**

**8 Hrs**

General mechanistic consideration – nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements, Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofman, Curtius, Schmidt, Shapiro reaction, Fries rearrangement. Reaction and mechanism of Diazo coupling, Glaser coupling, Heck reaction, McMurry reaction, Stille coupling, Suzuki coupling, Sonogashira reaction. Negishi and Hiyama coupling.

### UNIT-III

#### 4. Elimination Reactions:

5 Hrs

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.

#### 5. Oxidation Reactions:

7 Hrs

Introduction. Different oxidative processes. Hydrocarbons- alkenes, aromatic rings, saturated C-H groups (activated and unactivated). Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids. Amines, hydrazines, and sulphides. Oxidations with ruthenium tetroxide, iodobenzene diacetate and thallium (III) nitrate, DDQ, PCC, CAN, selenium dioxide, peroxyacids, DCC. Oxidation reactions with special emphasis on Baeyer-villiger reaction, Cannizzaro oxidation-reduction reaction,

### UNIT-IV

#### 6. Reduction Reactions:

10 Hrs

Introduction. Different reductive processes, Hydrocarbons- alkanes, alkenes, alkynes and aromatic rings, Carbonyl compounds – aldehydes, ketones, acids, ester and nitriles. Epoxides, Nitro, nitroso, azo and oxime groups, Hydrogenolysis. Sodium borohydride, sodium cyanoborohydride, LAH, diisobutylaluminum hydride, tin hydride, trialkyl tin hydride, trialkylsilanes, alkoxy substituted LAH, DIBAL, diborane, diisobutylborane, hexyl borane, 9-BBN, isopinocampheyl and diisopinocampheylborane. Reduction reactions with particular emphasis on Wolf-Kishner reduction, Clemmensen reduction.

#### Recommended Books:

1. Organic Reaction Mechanism by Jerry March, John Wiley Ed. 5, 2002.
2. Advanced Organic Chemistry by Francis Carey, Vol A and vol B

*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-II)*  
**CH 411/MHCH 411: Physical Chemistry-II**  
*Quantum Chemistry*

**45 Hrs.**

**Time: 4 Hrs/week.**

**Max. Marks: 37+13 (Internal Assessment)**

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of nine short questions carrying 1 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 7 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**1. Quantum Theory: Introduction and Principles**

**12Hrs**

Black body radiations, Planck's radiation law, photoelectric effect, Compton effect, De-Broglie hypothesis, the Heisenberg's uncertainty principle, Rydberg relation for explaining atomic spectrum of hydrogen. Bohr's Theory and its limitation solution of classical wave equation by separation of variables method.

**UNIT-II**

**2. Quantum mechanical operators**

**5 Hrs**

Operators and observations, normal and orthogonal functions, hermitian and unitary operators, introduction to differentiation and integration, Eigen value equation. Hamiltonian operator, interpretation of wave function, postulates of quantum mechanics.

**3. Applications of Quantum Postulates**

**7Hrs**

Solution of particle in one and three dimensional box, degeneracy, the linear harmonic oscillator, rigid rotators, quantization of vibrational and rotational energy levels, hydrogen atom.

**UNIT-III**

**3. Angular Momentum**

**5 Hrs**

Commutative laws, need of polar coordinates, transformation of Cartesian coordinate into polar coordinate, angular momentum of one particle system, orbital angular momentum, the ladder operator for angular momentum, spin angular momentum and their relations.

**4. The Approximate Methods**

**6 Hrs**

Need for approximation methods, Perturbation and Variation methods and their application to Helium atom.

**UNIT-IV**

**4. General Orbital Theory of Conjugated Systems**

**10Hrs**

Chemical bonding, linear combination of atomic orbital, overlap integral, coulomb's integral, bond order, charge density calculations for ethylene, allyl system, butadiene system, cyclo butadiene cyclopropenyl system.

**Recommended Books:**

1. Physical Chemistry, A Molecular Approach by MacQuarrie and Simon.
2. Quantum Chemistry, Ira N. Levine, Prentice Hall.
3. Quantum Chemistry, H. Eyring, Kimball and Walter.
4. Quantum Chemistry, Atkin.
5. Fundamentals of Quantum Chemistry, Anantharaman. R.



*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-II)*  
**CH 412/MHCH 412: Spectroscopy-B**  
*Techniques for Structure Elucidation of Inorganic Compounds*

60 hrs.

Time: 6 Hrs

Max. Marks: 56+19(Internal Assessment)

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of EIGHT questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of eight short questions carrying 1 Marks each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 12 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**1. Vibrational Spectroscopy**

15 hrs

**Theory of Infrared Absorption:** Harmonic and anharmonic oscillators, absorptions of radiation by molecular vibrations, selection rules, force constant, frequency of vibrational transitions of HCl, vibrations in a polyatomic molecule, 3N-6 and 3N-5 rules, types of vibrations, overtones, combination and difference bands, examples of CO<sub>2</sub>, SO<sub>2</sub>, and H<sub>2</sub>O, Fermi resonance, group vibrations.

**Raman Spectroscopy:** Introduction, selection rules, anisotropic polarizability, Stokes, anti-Stokes lines, vibrational Raman spectra of CO<sub>2</sub> and H<sub>2</sub>O, polarised and depolarised Raman lines, rule of mutual exclusion, vibronic coupling.

**Determination of IR/Raman Active Modes:** Significance of nomenclature: used to describe various vibrations, use of symmetry considerations to determining the number of active infrared and Raman lines (character tables to be provided in the Examination).

Sample handling. Factors affecting absorption frequencies. Interpretation and finger printing regions. Applications of Raman and I.R selection rules to the determination of Inorganic structure with special emphasis on:

- i) Metal carbonyls
- ii) NSF<sub>3</sub>
- iii) Geometrical isomerism – differentiation between Cis and trans [Co(bipy)<sub>2</sub>Cl<sub>2</sub>]Cl.
- iv) Structures of CO<sub>2</sub>, N<sub>2</sub>O, H<sub>2</sub>O, chlorocomplexes of mercury, cadmium and zinc, and octahedral complexes SiF<sub>6</sub><sup>2-</sup>, PF<sub>6</sub><sup>-</sup>, SF<sub>6</sub>.
- v) Changes in the spectra of donor molecules upon coordination with special emphasis on N, N-dimethylacetamide and DMSO with Fe<sup>3+</sup>, Cr<sup>3+</sup>, Zn<sup>2+</sup>, Pd<sup>2+</sup> and Pt<sup>2+</sup> ions. I.R spectroscopy and modes of coordination of SO<sub>4</sub><sup>2-</sup>, N<sub>2</sub>, O<sub>2</sub>, NO, CO<sub>3</sub><sup>2-</sup>, NO<sub>3</sub><sup>-</sup>.

**UNIT-II**

**2. Pure Rotational Spectra**

8

hrs Classification of molecules according to their moment of inertia. Rotational spectra of

diatomic molecules (rigid rotator), Intensities of spectral lines, isotopic substitution effects, non-rigid rotator, polyatomic linear and symmetric top molecules, Stark effect.

**3. Nuclear Quadruple Resonance Spectroscopy** **7 hrs**

Introduction, Experimental considerations, fundamentals of NQR spectroscopy, origin of EFG, measurement of energy differences between two nuclear spin states, the asymmetry parameters, effects of magnetic field, crystal field. Interpretation of spectra, application of the technique to halogen compounds (Organic), group elements, transition metals. Double resonance technique.

**UNIT-III**

**4. Photo Electron Spectroscopy** **8 hrs**

Introduction, excitation and ejection of electrons, electronic energy in atoms and molecules, core level PES, symmetry and molecular orbitals, molecular orbital diagrams of dinitrogen and dioxygen, their XPS spectra, Valence electron photoelectron spectroscopy, Franck Condon principle, dissociation, predissociation, change of shapes of molecules on excitation.

**5. Mössbauer Spectroscopy** **8hrs**

Principle, experimental considerations, conditions of MB Spectra, the spectrum and its parameters, simple spin states ( $I = \frac{1}{2}, 3/2$ ), higher spin states ( $I > 3/2$ ), magnetic splitting significance of parameters obtained from spectra, quadruple splitting, additive model, interpretation of MB Spectra of  $^{57}\text{Fe}$ ,  $^{119}\text{Sn}$ . Application to biological systems, surface study, and compounds of group elements.

**UNIT-IV**

**6. Electron Spin Resonance Spectroscopy** **14hrs**

Introduction, principle, brief instrumentation of spectrum, hyperfine splitting in isotropic systems involving more than one nucleus, ESR spectrum of benzene radical anion, methyl radical,  $\text{CH}_2\text{OH}$ ,  $\text{H}_3\text{CCH}_2$  radical, cyclopentadienyl, cycloheptatrienyl radical, pyrazine anion, pyrazine anion with  $^{23}\text{Na}$  and  $^{39}\text{K}$  counter ion and p-benzosemiquinone, DPPH, Naphthalene. Factors affecting magnitude of g values, zero field splitting, and Kramer's degeneracy. Qualitative survey of EPR spectra of first row transition metal ion complexes ( $d^1, d^2, d^3$ , low spin  $d^5$ , high spin  $d^6, d^7, d^9$  system). Spectra of triplet states, rate of electron exchange, double resonance (ENDOR, ELDOR)

**Books Recommended:**

- 1) R. S. Drago, "Physical Methods in Chemistry". W.B Saunders Company.
- 2) C. N. Banwell, "Fundamentals of Molecular Spectroscopy".
- 3) R. V. Parish, "NMR, NQR, EPR & Mossbauer spectroscopy in Inorganic Chemistry". Ellis Horwood, London, 1990.
- 4) G. M. Barrow, "Introduction to Molecular Spectroscopy".
- 5) E. A. Ebsworth, S. Craddock and D. W. H. Rankin, "Structural methods in Inorganic Chemistry". Blackwell Scientific Publications (1991).
- 6) C. N. R. Rao and J. R. Ferraro, "Spectroscopy in Organic Chemistry, Vol. I". Academic Press (1971)
- 7) Walker and Straughan, "Spectroscopy, Vol I and III".

*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-II)*  
**CH 413/MHCH 413: Organic Synthesis-III**  
*Supramolecular, Reactive Intermediates and Disconnections*

**45 Hrs.**

**Time: 4 Hrs/week.**

**Max. Marks: 37+13 (Internal Assessment)**

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of nine short questions carrying 1 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 7 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**1. Supramolecular Chemistry-I**

**(a) Concepts**

**3Hrs**

Definition and Development of Supramolecular Chemistry, classification of Supramolecular Host-Guest compounds, Pre- organization and Complementarily, Receptors, Nature of Supramolecular interactions.

**(b) Binding of anions and neutral molecules**

**8Hrs**

Biological anion receptors, concepts on anion host design, Fromcation to anion hosts-a simple change in pH, Guanidinium- based receptors, Neutral receptors, organometallic receptors, coordination interactions. Inorganic solid state clathrate compounds, solid state clathrates of organic hosts, intracavity complexes of neutral molecules, supramolecular chemistry of fullerenes.

**UNIT-II**

**2. Supramolecular Chemistry-II**

**(c) Cation Binding Host**

**5Hrs**

Crown ethers, Lariat ether and Podands, Cryptands, spherands, selectivity, Macro cyclic, Macrobicyclic and Template effects, soft ligands, calixarenes, carbon donor and - acid ligands, siderophores.

**(d) Crystal Engineering and Molecular Devices**

**6Hrs**

Concepts, crystal structure prediction, Crystal Engineering with hydrogen bonds, weak hydrogen bonds, hydrogen bonds to metals and metal hydrides,  $\pi$ -  $\pi$ stacking, coordination polymers. Introduction, Supramolecular photochemistry, molecular electronic devices: Switches, wires and rectifiers, machines based on catenanes and rotaxanes.

### UNIT-III

#### 3. Organic Reactive Intermediates-I

12Hrs

**(a) Carbanions:** Chemistry of enolates and enamines, kinetic and thermodynamic enolates, Lithium and boron enolates in aldol and Michael reactions, alkylation and acylation of enolates, Nucleophilic additions to carbonyls and stereochemical aspects through various models (Cram's / Cram chelation / Felkin-Anh models)

**(b) Carbocations:** Structure and stability of carbocations, classical and non classical carbocations, Neighbouring group participation.

**(c) Carbenes and Nitrenes:** Structure, generation addition and insertion and rearrangement reactions of carbenes such as Wolff rearrangement. Generation of ylids by Wolff decomposition. Structure, generation and reactions of nitrene and related electron deficient nitrogen intermediates.

### UNIT-IV

#### 4. Organic Reactive Intermediates

06Hrs

**(d) Ylids:** Chemistry of Phosphorous and Sulphurylids-Wittig and related reactions, Peterson olefination etc.

**(e) Radicals:** Generation of radical intermediates and its addition to alkenes, alkynes for C-C bond formation and Baldwin's rule. Fragmentation and rearrangement reactions like decarboxylation, McMurry coupling etc.

#### 5. Disconnection approach

05Hrs

An introduction to synthons and synthetic equivalents, disconnection approach, functional group interconversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis.

#### Recommended Books :

1. J.W Steed and J.L Atwood, Supramolecular chemistry, John Wiley & Sons, Ltd. New York.
2. Designing Organic Synthesis, S. Warren, Wiley
3. Organic Synthesis- Concepts, Methods and Starting Materials, J. Fuhrhop and G. Penzillin, Verlag VCH.
4. Advanced Organic Synthesis Part A and B, F.A. Carey and R. J. Sundberg, Plenum Press.
5. Principles of Organic Synthesis, R. Norman and J. M. Coxon, Blackie Academic & Professional
6. *Modern Methods of Organic Synthesis* Cambridge University Press (1971). Carruthers,
7. Reactive Intermediates, Gilchrist and Rees

M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-II)  
CH 414(a)/MHCH 414 (a): Mathematics for Chemists

For Non-Medical Students

30 hrs.

Time:2HrsMax.

Marks: 18+07(Internal Assessment)

Instructions for paper setters and candidates

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of eight short questions carrying  $\frac{1}{2}$  Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry  $3\frac{1}{2}$  Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

UNIT-I

1. Trigonometry

7 Hrs

Definition of sin, cos, tan, cot, sec, cosec functions with the help of unit circle, values of sin x cos x for  $x = 0, \pi/6, \pi/3, \pi/2$ . Meaning of a trigonometrical identity. The following identities (no need of derivation and proof. However, application has to be emphasized).

$$\cos^2 x + \sin^2 x = 1$$

$$\sin(x+2\pi) = \sin x$$

$$\cos(x-2\pi) = \cos x$$

$$\cos(-x) = \cos x; \sin(-x) = -\sin x$$

$$\sin(\pi-x) = \sin x; \cos(\pi-x) = -\cos x$$

$$\sin(\pi+x) = -\sin x; \cos(\pi+x) = -\cos x$$

$$\sin 2x = 2 \sin x \cos x$$

$$\cos 2x = \cos^2 x - \sin^2 x$$

$$\cos 2x = 2\cos^2 x - 1$$

$$\tan(x) = \frac{\sin x}{\cos x}$$

$$\tan(x) = -\tan(\pi-x); \tan\left(\frac{x}{2} - \frac{\pi}{2} - x\right) = \cot x$$

$$\tan(\pi-x) = -\tan x$$

$$\tan 2x = \frac{2 \tan x}{1 - \tan^2 x}$$

UNIT-II

2. Determinants and Matrices

5 Hrs

Definition and expansion properties of determinants, product of two determinants of 3<sup>rd</sup> order.

Introduction to various terms Matrix, row, column, diagonal unit. Sub, square, equal matrices, null, symmetric, order of, character of, transpose of, adjoint of, inverse of matrices. Addition multiplication, diagonalization, similarity transformation of matrices, characteristic equation statement of Cayley-Hamilton theorem. Rank of matrix, condition of consistency of a system of linear equations. Eigen vectors and Eigen values using matrices.

### **UNIT-III**

#### **3. Differential Calculus**

**8 Hrs**

Differentiation of standard functions, theorems relating to the derivative of the sum, difference, product and quotient of functions, derivative of trigonometric functions, inverse trigonometric functions, logarithmic functions and exponential functions, differentiation of implicit functions, logarithmic differentiation.

### **UNIT-IV**

#### **4. Integral Calculus (10 Hrs.)**

Integration as an inverse of differentiation summation, area under a curve, indefinite integrals of standard forms, method of substitution, method of partial fractions, integration by parts, definite integrals, reduction formulae, definite integrals of limit of a sum and geometrical interpretation.

#### **Books Recommended:**

1. Santi Narayan – Differential Calculus.
2. Santi Narayan - Integral Calculus.
3. B.S. Grewal – Higher Engineering Mathematics.
4. Joseph B. Dence – Mathematical Techniques in Chemistry.
5. Margenau and Murphy, the Mathematics of Physics and Chemistry.
6. B.L. Moncha and H.R. Choudhary – A Text Book of Engineering Mathematics.

*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-II)*  
**CH 414(b)/MHCH 414(b): Biology for Chemists**

**For Medical Students**

**30 hrs.**

**Time: 2 Hrs**

**Max. Marks: 18+07 (Internal Assessment)**

**Instructions for paper setters and candidates**

- I. Examiner will set total of TEN questions.
- II. Section-A will be of the First Question consisting of six short answer type questions of  $\frac{1}{2}$  mark each covering the whole syllabi. This will be a compulsory question. The total weightage will be 3 Marks.
- III. Section B, C and D will consist of 3 questions from each Unit-I, II and III respectively. Each question will be carrying 3 marks and the students are required to attempt Five questions in all, at least ONE question from each unit. The weightage of this section will be 15 Marks

**UNIT-I**

**1. The Organisation of Life**

**10Hrs**

Biologically important molecules: Carbohydrates, lipids, proteins and nucleic acids.

The life of cells – The cell theory, general characteristics of cells, difference between prokaryotic and eukaryotic cells, difference between plant and animal cells, cell organelles.

Tissues, organs and organ systems: Animal tissues; epithelial tissues, connective tissues, muscle tissue, nervous tissue and neoplasias; plant tissue: meristematic tissue, permanent tissues.

**UNIT-II**

**2. Genetics**

**10Hrs**

The basic principle of heredity: Mendel's law, monohybrid cross, dihybrid cross.

DNA – Double helix structure and replication.

Gene expression: Transcription and translation, genetic code.

**UNIT-III**

**3. The Diversity of Life**

**10Hrs**

The classification of Living things – Criteria of classification, Whittaker's systems of classification, their characteristics with an example of each.

Viruses, structure of Viruses.

**Book Recommended:**

***Academic Session: 2020-21***

1. Cord Biology - South Western Educational Publications, Texas, 2000.



*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-II)*  
**CH 415/MHCH 415: Physical Chemistry Practical-I**

**Max. Marks: 75+25(Internal Assessment)**

**Labs Hrs.: 60**

1. To determine the strength of given acid by *pH* metrically.
2. To determine dissociation constant of given acid *pH* metrically
3. Titration of weak acid conductometrically
4. Titration of strong acid conductometrically
5. To determine dissociation constant of given acid conductometrically
6. Determine the dissociation constant of acetic acid in DMSO, DMF, dioxane by titrating it with KOH.
7. Determine the activity coefficient of an electrolyte at different molalities by e.m.f. measurements.
8. Compare the cleansing powers of samples of two detergents from surface tension measurements.
9. Determine the specific refraction, molar refraction and atomic parachor with the help of Abbe's refractometer.
10. To study the distribution of benzoic acid between benzene and water.
11. Determine the equilibrium constant of reaction  $K_1 + I_2 \rightarrow KI_3$  by distribution law and hence Find the value of *GO* of the above reaction
12. Compare the relative strength of  $CH_3COOH$  and  $ClCH_2COOH$  from conductance measurements.
13. Determine the solubility (g/litre) of sparingly soluble lead sulphate from conductance measurements.
14. Titrate a given mixture of HCl and  $CH_3COOH$  against NaOH solution conductometrically..
15. Compare the relative strength of:
  - i) HCl
  - ii)  $H_2SO_4$by following the kinetics of inversion of cane sugar polarimetrically.

*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-II)*  
**CH 416/MHCH 416: Inorganic Chemistry Practical-II**

**60 hrs.**

**Time: 6 Hrs.**

**Max. Marks: 75+25 (Internal Assessment)**

**(Any 8 Complexes.)**

1. Preparation of  $\text{Co}(\text{acac})_3$ , its characterization using NMR, IR, UV-Vis and analysis of Cobalt (ref. J. Chem. Edu., 1980, 57, 7, 525)
2. Preparation of  $\text{Co}(\text{acac-NO}_2)_3$ , its characterization using NMR, IR, UV-Vis and analysis of Cobalt. (ref. J. Chem. Edu., 1980, 57, 7, 525)
3. Preparation of  $[\text{Fe}(\text{H}_2\text{O})_6][\text{Fe}(\text{N-salicylideneglycinato})_2]_2 \cdot 3\text{H}_2\text{O}$ , its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Iron.(ref. InorganicaChimicaActa, 1977, 23, 35).
4. Preparation of  $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$ its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Nickel and  $\text{NH}_3$ . (ref. Marr and Rockett, 1972).
5. Preparation of  $[\text{Ni}(\text{ethylenediamine})_3]\text{Cl}_2$  its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Nickel. (ref. Marr and Rockett, 1972, page 270).
6. Preparation of  $[\text{Fe}(\text{NO})(\text{S}_2\text{CN}(\text{Et})_2)_2]$  its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Fe(II). (ref. Marr and Rockett, 1972, page 262, J. Chem. Soc. 1962, 84, 3404).
7. Preparation of octahedral and tetrahedral complexes of dichlorodipyridylcobalt(II), differentiate them using IR, UV and magnetic properties. Estimate Co(II) from one of them. (ref. Marr and Rockett, 1972, page 375, Inorganic Chemistry, 1966, 5, 615).
8. Preparation of  $\text{VO}(\text{acac})_2$ and its piperidine complex, characterize using IR, UV and magnetic moment. Estimate for V(IV). (ref. Marr and Rockett, 1972, 243).
9. Preparation of diaquotetraacetataocopper(II), magnetic susceptibility IR and UV-Vis, analysis of Copper(II).
10. Preparation of cis- and trans- potassium dioxalatodiaquochromate(III). Interpretation of IR, UV and magnetic properties.Estimation of Chromium. (ref. Marr and Rockett, 1972, page 386).
11. Preparation of  $\text{HgCo}(\text{NCS})_4$ , its IR and measure its magnetic moment. (ref. Marr and Rockett, 1972, page 365).
12. Preparation of sodium tetrathionate, interpretation of its IR and analysis using potassium iodate. (ref. Marr and Rockett, 1972, page 214).

13. Preparation of Potassium dithionate, interpretation of its IR and analysis using potassium iodate. (ref. Marr and Rockett, 1972, page 214).
14. Preparation of bis(acetylacetonato)copper(II), UV-Vis, and IR, magnetic studies, Demonstration of Jahn Teller effect by solution spectral studies. (ref. Bull. Chem. Soc. Japan, 1965, 29, 852).
15. Preparation of salicylamide complexes of Copper(II). IR, UV, magnetic data and analysis of Cu(II). (ref. Indian J. of Chem., 1977, 15A, No. 5, 459; *ibid*, 1971, 9, 1396).
16. To prepare a macrocyclic ligand 5,7,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradeca-4,11-dienedi(hydrogeniodide) and its complex with Ni(II). Study IR, NMR and UV-Vis of ligand and complex and magnetic properties of complex. To analyze for Ni and I. (J. Chem. Edu. 1977, 79, 581).
17. Preparation and resolution of tris (ethylenediamine) cobalt (III). UV-Vis, NMR, IR, optical rotation of the resolved complexes. ((ref. Marr and Rockett, 1972, page 386).

**Recommended Book:**

1. B.N. Figgis, Introduction to Ligand Field, Wiley Eastern.
2. A.B.P. Lever, Inorganic Electronic Spectroscopy, Elsevier.
3. A.Earnshaw, Introduction to Magnetochemistry, Academic Press.
4. J.E. Huheey, Inorganic Chemistry Principles of Structure and Reactivity, Harper Interscience.
5. R.S. Drago, Physical Method in Chemistry, W.B.Saunders Company.
6. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Wiley Int

# *Semester-III*

*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-III)*

**CH 417/MHCH 417: Inorganic Chemistry-III**

*Bioinorganic and Metal Clusters*

**45 Hrs.**

**Time: 4 Hrs/week.**

**Max. Marks: 37+13 (Internal Assessment)**

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of nine short questions carrying 1 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 7 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**1. (a) Bioinorganic Chemistry**

**12**

**Hrs** Periodic survey of essential and trace elements, biological importance and relative abundance, Na<sup>+</sup>/ K<sup>+</sup> ion pump and its mechanism.

Porphyrine and metalloporphyrins, Oxygen carriers/storage-Hb and Mb: Structure and mechanism of their function, cooperativity and Bohr effect. Synthetic models of Hb, Cyanide, phosphine and carbon monoxide poisoning.

Inhibition and poisoning by ligand and metal ions, hemocyanin and hemerythrin, models of iron, coal and copper.

Bioenergetic and ATP cycle process coupled to phosphate hydrolysis, Nucleotide transfer-DNA polymerase, phosphate transfer pyruvate kinase, phosphoglucomutase, creatin kinase, ATPase.

**UNIT-II**

**1. (b) Bioinorganic Chemistry**

**11 Hrs**

Photosynthesis and respiration - chlorophyll : structure, function and its synthetic model. Xanthine oxidase, Gout Disease and its remedy.

Enzymes and their functioning, Bioredox agents, Zn-enzymes carboxipeptidase, carbonic anhydrase, superoxide dismutase, peroxidases and catalases,

Vitamin B<sub>12</sub> coenzyme, structure, function and "Mn" mechanism and its application in organic synthesis, intake of alcohol and its remedy.

Cytochromes-structure and function, Cytochrome P<sub>450</sub> enzymes.

Ferredoxins and rubredoxins their structure and function. Abiological and biological N<sub>2</sub> fixation and mechanism.

### UNIT-III

#### 1. (c) Bioinorganic Chemistry

11 Hrs

Ferritin, transferrin and siderophores and their structure and function.

Availability, competition, toxicity and nutrition of Iron, metal deficiency and diseases, toxic effects of antibiotics, chelate therapy, synthetic metal chelates as antimicrobial agents.

Calcium in living cell, transport and regulation and its mechanism.

Molecular aspects of intramolecular processes and their mechanisms.

#### 2. Metal Clusters

##### (a) Reaction at Coordinated ligands

The role of metal ions in the hydrolysis of amino acid esters, peptides, and amides Molecular orbital concept of role of metal ions participation, Modified aldol condensation, Imine formation, Template and Macrocyclic effect in detail.

### UNIT-IV

#### (b) Metal to Metal Bonds and Metal atom Clusters

11 Hrs

Metal carbonyl clusters, isoelectronic and isolobal relationship, high nuclearity carbonyl clusters (HNCC), Structural Patterns, synthetic methods, heteroatoms in metal atom clusters

Carbide and nitride containing clusters, electron counting scheme for HNCC's, the capping rule, HNCC's for Fe, Ru, Os, Co, Rh, Ir, Ni, Pd, Pt.

Lower halides and chalcogenides clusters, octahedral metal halides and chalcogenides clusters ( $M_6M_8M_6M_{12}$  type).

Several phases, triangular clusters and solid state extended arrays. Compound with M-M multiple bonds, major structural types, quadruple bonds, other bond orders.

Intracluster relation of clusters to multiple bonds and one dimensional solids.

#### Books Recommended:

1. Principles of Bioinorganic Chemistry, S. J. Lippard and Berg, University Science Books.
2. J.E. Huheey : Inorganic Chemistry III & IV Ed. Pearson Education Asia – (2002).
3. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 5<sup>th</sup> Edition.
4. Purcell and Kotz: Inorganic chemistry. W. B. Saunders and Co., London
5. Bioinorganic Chemistry by D. Banerjee

*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-III)*  
**CH 418/MHCH 418: Organic Synthesis-IV**  
*Natural Products*

**45 Hrs.**

**Time: 4 Hrs/week.**

**Max. Marks: 37+13 (Internal Assessment)**

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of nine short questions carrying 1 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 7 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**1. Studies on Biosynthetic Pathways of Natural Products**

**8 Hrs**

a) The acetate hypothesis, poly-ketoacids, their addol type cyclisations and meta orientations of hydroxyl groups in naturally occurring phenols.

b) Isoprene rule, mechanism of formation of mevalonic acid from acetyl coenzyme, Biogenetic isoprene rule. Geranyl pyrophosphates and its conversion into alphapinene, thujene and borneol. Farnesyl pyrophosphate, geranyl, geranyl pyrophosphate and mechanistic considerations for their interconversions into cadinene and abietic acid.

**2. Terpenoids**

**4 hrs**

General classification, General Methods of structure determination, Chemistry of Camphor, Abietic acid, Santonin biosynthetic studies on tri and tetra terpenoids.

**UNIT-II**

**3. Carbohydrates**

**6 Hrs**

Conformation of monosaccharides, structure and functions of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol, amino sugars, N-acetylmuramic acid, sialic acid, disaccharides and polysaccharides. Structural polysaccharides-cellulose and chitin. Storage polysaccharides – cellulose and chitin. Storage polysaccharides-starch and glycogen. Structure and biological functions of glucosaminoglycans or mucopolysaccharides. Carbohydrate metabolism-Kreb's cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis, pentose phosphate pathway.

**4. Amino-acids, Peptides and Proteins**

**5 Hrs**

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures.  $\alpha$ -helix,  $\beta$ -sheets, super secondary structure, triple helix structure of collagen, Tertiary structure of protein-folding and domain structure. Quaternary structure.

Amino- acid metabolism-degradation and biosynthesis of amino acids, sequence determination: chemical/enzymatic/mass spectral, recemization/detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH)

### **UNIT-III**

#### **5. Nucleic Acids** **5 Hrs**

Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis for heredity, and overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and trinucleoside.

#### **6. Steroids** **3 Hrs**

General biosynthetic studies on steroids, chemistry of Cholesterol, cortisone, progesterone, oestrone, transformations in steroid molecules.

#### **7. Alkaloids** **3Hrs**

Classification, chemistry of nicotine, quinine, papaverine, morphine and reserpine.

### **UNIT-IV**

#### **6. Haemin and Chlorophyll** **5Hrs**

Structure and synthesis of Porphyrins. Chemistry of Haemin and chlorophyll.

#### **7. Antibiotics** **3Hrs**

Introduction, chemistry of pencillins, streptomycines, chloromphenicol, tetracyclins.

#### **8. Prostaglandins** **3Hrs**

General study, nomenclature, structure of PGE and synthesis of PGE1, PGE2, PGF2x

#### **Books Recommended:**

1. Primary Metabolism: A Mechanistic Approach by J. Staunton, Oxford University Press, 1978.
2. Secondary Metabolism by J. Mann, Oxford University Press, Oxford, 1980.
3. Natural Product Chemistry - A mechanistic, Biosynthetic and Ecological Approach by Kurt B. G. Torssell, Swadish Pharmaceutical Society, 1997.
4. Principles of Biochemistry by A. L. Lehninger, CBS Publishers, New Delhi.
5. Fundamental of Biochemistry by D. Voet, J.G. Voet and C.W. Pratt, John Willey & Sons Inc., New York, 1999.



*M.Sc. Chemistry (Semester- III)*  
**CH419: Physical Chemistry-III**  
*Electrochemistry and Chemical Dynamics*

**60Hrs.**

**Time: 8 Hrs.**

**Max. Marks: 56+19 (Internal Assessment)**

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of EIGHT questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of eight short questions carrying 1 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 12 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**1.Electrochemistry**

**15Hrs**

Electrochemistry of solutions, Debye-Huckel-Onsager treatment and its extension, ion-solvent interactions, Thermodynamics of electrified interface equation, Derivation of electro-capillarity, Lipmann equation(surface excess), method of determination, structure of electrified interfaces, Helmholtz-Perin, Guoy-Chapmann, Stern models, overpotential, exchange current density, derivation of Butler-Volmer equation, Tafel plot.

Semiconductor interface theory of double layer at semiconductor electrolyte solution interface, structure of double layer interfaces, effect of light at semiconductor solution interface. Introduction to corrosion, forms of corrosion, corrosion monitoring and prevention.

**UNIT-II**

**2.(a)Chemical Dynamics**

**15Hrs**

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius theory and activated complex theory, ionic reactions, kinetic salt effects,, treatment of uni molecular reactions, Lindemann-Hinshelwood theory.

**UNIT-III**

**2.(b)Chemical Dynamics**

**15Hrs**

Dynamic Chain (hydrogen bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), Photochemical reactions between hydrogen-bromine and hydrogen-chlorine, oscillatory reactions (Belousov-Zhabotinsky reactions), Homogeneous catalysis and kinetics of enzyme

reactions, general features of fast reactions, study of fast reactions by flow method, , relaxation method, flash photolysis, nuclear resonance.

#### **UNIT-IV**

### **3.Voltmometry and Polarography**

**15Hrs**

Polarography, polarographic cells, polarogram, interpretation of polarographic waves, equation for the polarographic waves, effect of complex formation on polarographic wave, polarograms for irreversible reactions, dropping mercury electrode, current variations during life time of a drop, merits and demerits of dme, polarographic diffusion currents, Ilkovic equation, capillary characteristics, temperature, polarograms for mixture of reactants, anodic and cathodic waves, factors affecting polarographic currents, applications of polarography, treatment of data, organic and inorganic polarographic analysis, voltammetry at solid electrodes, cyclic voltammetry and interpretation of data, , pilot-ion and standard addition method for quantitative analysis.

#### **Books Recommended:**

1. Chemical Kinetics, K. J. Laddler, McGraw-Hill
2. Modern Electrochemistry Vol.1,2,3, J. Bochriss and A.K.N. Reddy
3. Fundamentals of electrochemistry; P. Monk
4. Principles of Instrumental Analysis; Skoog, West; Saunders Publications

*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-III)*  
**CH 420/MHCH 420: Organic Synthesis-V**  
*Pericyclic and Photochemistry*

45 Hrs.

Time: 4 Hrs/week.

Max. Marks: 37+13 (Internal Assessment)

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of nine short questions carrying 1 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 7 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**1. (a) Pericyclic Reactions**

**12 Hrs**

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene, allyl system, classification of pericyclic reactions FMO approach. Woodward-Hoffmann correlation diagrams method and Perturbation of molecular orbital (PMC) approach for the explanation of pericyclic reactions under thermal and photo-chemical conditions.

Electrocyclic reactions – conrotatory and disrotatory motions,  $4n$ ,  $4n+2$ , allyl systems secondary effects. Cycloadditions – antarafacial and suprafacial additions, notation of cycloadditions ( $4n$ ) and ( $4n+2$ ) systems with a greater emphasis on (2+2) and (4+2) cycloaddition-stereochemical effects and effects of substituents on the rates of cycloadditions, 1,3-dipolar cyclo-additions and cheletropic reactions.

**UNIT-II**

**1. (b) Pericyclic Reactions**

**10 Hrs**

Sigmatropic Rearrangements-suprafacial and antarafacial shifts [1,2]- sigmatropic shifts involving carbon moieties retention and inversion of configuration, (3,3) and (5,5) sigma-tropic rearrangements, detailed treatment of Claisen and Cope rearrangements, fluxional tautomerism, aza-cope rearrangements, introductions to Ene reactions, simple problems on pericyclic reactions. Electrocyclic rearrangement of cyclobutenes and 1,3cyclohexadienes.

**UNIT-III**

**2. Photochemistry**

**(i) Photochemical Reactions**

**3 Hrs**

Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

**(ii) Determination of Reaction Mechanism**

**3 Hrs**

Classification, rate constants and life times of reactive energy states –determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions.

Types of photochemical reactions – photodissociation, gas-phase photolysis.

**(iii) Photochemistry of Alkenes**

**5 Hrs**

Intramolecular reactions of the olefinic bond – geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1, - dienes.

**UNIT-IV**

**(iv) Photochemistry of Carbonyl Compounds**

**6 Hrs**

Intramolecular reactions of carbonyl compounds – saturated, cyclic and acyclic,  $\beta$ ,  $\gamma$ - unsaturated and  $\alpha,\beta$ -unsaturated compounds, Cyclohexadienones. Intermolecular cycloaddition reactions – dimerisations and oxetane formation.

**(v) Photochemistry of Aromatic Compounds**

**3 Hrs**

Isomerisations, additions and substitutions.

**(vi) Miscellaneous Photochemical Reactions**

**3 Hrs**

Photo-Fries reactions of anilides. Photo-Fries rearrangement. Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision.

**Books Recommended:**

1. Pericyclic reactions: A Mechanistic study by S. M. Mukherji
2. The Conservation of Orbital Symmetry by R. B. Woodward and R. Hoffman
3. Organic Photochemistry – Chapman and Depuy.
4. Organic Photochemistry – W.H. Horsepool.
5. Photochemistry of Excited States – J.D. Goyle.
6. Fundamentals of Photochemistry by K.K. Rohtagi Mukherji

*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-III)*  
**CH 421/MHCH 421: Physical Chemistry-IV**  
*Analytical Techniques*

**45 Hrs.**

**Time: 4 Hrs/week.**

**Max. Marks: 37+13 (Internal Assessment)**

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of NINE questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of nine short questions carrying 1 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 7 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**1.(a) Potentiometric Methods**

**7Hrs**

Reference electrodes: Calomel electrodes, silver- silver chloride electrodes, precautions in the use of reference electrodes, metallic indicator electrodes and its types, metallic redox indicators, membrane indicator electrodes, classification of membranes, properties of ion-selective electrodes, the glass electrodes for pH measurement, composition and structure of glass membrane, the hygroscopicity of glass membrane, conduction across glass membrane, the membrane potential, the boundary potential, the potential of glass electrode, the alkaline and error, the glass electrodes for other cations, crystalline membrane electrode and their conductivity, the fluoride electrode, the electrode based on silver salts.

**1.(b) Potentiometric Methods**

**4Hrs**

Direct potentiometric measurement, sign conventions, the electrode calibration method, calibration curves for concentration measurements, potentiometric pH measurements with a glass electrode, errors affecting pH measurements with glass electrode.

**UNIT-II**

**2. Thermal Methods**

**06Hrs**

Thermogravimetric methods(TG) :Instrumentation, The balance, Furnace, instrument control, applications, Differential thermal analysis(DTA), instrumentation, general principles, applications, Differential scanning calorimetry(DSC), applications.

**3. Solid State Chemistry**

**05Hrs**

Types of solids, band and band theories, point defects in metals and ionic compounds, energy and entropy defects and their concentration, diffusion and electrical conduction via defects, non-

stoichiometric defects, color centers and electrical properties of alkali metals halides, impurity semi-conductors reactions in organic solids, photochemical reactions, sintering solid state reactions, decomposition and dehydration reaction

### **UNIT-III**

#### **4.Coulometric Methods**

**11Hrs**

Current-Voltage relationships during an electrolysis, operation of a cell at a fixed applied potential, initial thermodynamic potential, estimation of required potential, current changes during an electrolysis at constant applied potential, potential changes during an electrolysis at constant applied potential, constant current electrolysis, electrolysis at a constant working electrode potential, An introduction to coulometric methods of analysis, units for quantity of electricity, types of coulometric methods, applications, coulometric titrations, applications of coulometric titrations, comparison of coulometric and volumetric titrations.

### **UNIT-IV**

#### **5. An Introduction to Chromatographic Separations**

**6Hrs**

General description of chromatography, classification of chromatographic methods, Elution chromatography on columns, chromatograms, effect of migration rates and band broadening on resolution, Migration rates of species, partition coefficients, retention time, relationship between retention time and partition coefficients, the rates of solute migration(capacity factor), differential migration rates, the shape of chromatographic peaks, methods for describing column efficiency, definition of plate height, experimental evaluation of H and N, kinetic variables affecting band broadening, relationship between plate height and column variables.

#### **6. Gas Chromatography**

**6Hrs**

Principles of Gas-Liquid chromatography, Instrumentation: carrier gas supply, sample injection system, column configuration and column ovens, detectors, Flame ionization detectors (FID), Thermal conductivity detectors (TCD), Thermionic detectors (TID), Electron capture detectors (ECD), Atomic emission detector (AED), Gas chromatographic columns and stationary phase: packed column, open tubular column, adsorption on column packing, stationary phases.

#### **Books Recommended:**

- 1.Solid State Chemistry : A.R.WEST
- 2.Principles of Instrumental Analysis: Skoog and West
- 3.Principles of Instrumental Analysis : Willard, Merit and Dean
4. Solid state physics: A J Dekker, Macmillan Publishers
5. Principles of physical chemistry: Puri, Sharma, Pathania.
6. Chemistry of solid state: W E Garner, Butterworth

**Academic Session: 2020-21**

*M.Sc. Chemistry (Semester-III)*  
**CH422: Organic Lab-II**  
*Advanced Organic Chemistry Practical*

**60 hrs.**

**Time: 6 Hrs/week.**

**Max. Marks: 75+25 (Internal Assessment)**

1. Synthesis and Reactivity of benzalacetophenone
  - a. Bromination (Electrophilic additions) & subsequent debromination (Elimination)
  - b. Epoxidation (Cycloaddition, nucleophilic) and ring opening with hydroxide ion.
  - c. Michael addition of aniline.
  - d. Conversion of benzalacetophenone to its oxime (nucleophilic addition at C=O)
  - e. Conversion of oxime to amide (Beckmann rearrangement) and oxazole  
(Understand the reactivities at conjugated C=O and C=C) bond.
1. Synthesis of Cyclohexene from cyclohexanol and its conversion to 1, 2- *cis* and 1, 2- *trans*-cyclohexanediols.
  - a. Epoxidation with peracid (Cycloaddition) and *anti*- ring opening with sodium hydroxide to *cis*- cyclohexane -1, 2- diol.
  - b. Dihydroxylation with KMnO<sub>4</sub>  
(Mechanism of *syn*- and *anti*-cyclohexane-1,2-diol)
2. Preparation and characterization of the Aldol-dehydration products from various combinations of aromatic aldehydes and ketone. Effect of substituents on aromatic aldehydes on the product distribution.
  - a. Aldehyde: benzaldehyde, 4-methylbenzaldehyde, 4-methoxybenzaldehyde.
  - b. Ketone: acetone, cyclopentanone, cyclohexanone (Book 4).

**Recommended Books:**

1. An Introduction to Modern Experimental Organic Chemistry, R.M. Roberts, J.C. Gilbert, L.B. Rodewald and A.S. Wingrove, Holt Rinehart and Winston Inc, New York. 1969.
2. Vogel's Text Book of Practical Organic Chemistry.
3. Laboratory Experiments on Organic Chemistry, R. Edemas, J.R. Johnson and C.F. Wilcox, The Macmillan Limited, London, 1970.
4. Modern Projects and Experiments in Organic Chemistry, J.R. Mohrig, C.N. Hammonad, P.F. Schatz and T.C. Morrill, W.H. Freeman and Company, New York 2003.

*M.Sc. Chemistry (Semester-III)*  
**CH423: Physical Chemistry Lab-II**  
*Electroanalytical Techniques*

**Max. Marks: 75+25 (Internal Assessment)**

**Labs Hrs.: 60**

1. To determine the partial molar volume of  
(a) Glycine (b) Urea using dilatometer
2. To determine the partial molar volume of  
(a) methanol (b) n-propanol using dilatometer
3. To determine the surface tension (double capillary) of mixture of solid and water by differential method and hence find out parachor of the mixture.
4. To determine the specific and molar refractivity of n-propanol, butanol, hexane and carbon tetrachloride and calculate refraction equivalents of C, H and Cl.
5. To determine the molar refractivity of water, DMF, dioxane and mixtures of water, DMF, water-Dioxane and verify the refractivity rule. Predict about the interactions between components of mixture by plotting graph between refractive index and mole fraction.
6. To determine the equivalent conductance of weak electrolyte acetic at infinite dilution using Kohlrausch law.
7. Determine equivalent conductance of strong electrolyte at several concentrations and hence verify Onsager's equation.
8. Determine equivalent conductance of weak electrolyte, say, acetic acid at different concentrations and hence test validity of Ostwald's dilution law. Also determine dissociation constant of the electrolyte.
9. To determine dissociation constant of a dibasic acid potentiometrically.
10. To study complex formation between Fe(III) and salicylic acid and find out the formula of the complex spectrophotometrically.
11. To determine the formula of the complex ion formed between Fe(III) and Thiocyanate ion by Job's method.
12. To study the kinetics of hydrolysis of crystal violet spectrophotometrically.
13. To determine the pH of a buffer solution (pH less than 8) using a quinhydrone electrode.
14. To determine the pH of various mixtures of sodium acetate and acetic acid in aqueous solution and hence determine the dissociation constant of the acid.
15. Titrate potentiometrically Zn (II) by  $K_4Fe(CN)_6$  and verify the composition of the complex  $K_2Zn_3 [Fe(CN)_6]_2$
16. Determination of nitrite in water spectrophotometrically.
17. Determination of molecular weight of polymers by Turbiditymetry.
18. Determine the molar refraction of a solid substance by dissolving it in a solvent and its refractive index.



# *Semester-IV*

*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-IV)*  
**CH424/MHCH 423: Inorganic Chemistry-IV**  
*Advanced Inorganic Chemistry*

**60 hrs.**

**Time: 8 Hrs.**

**Max. Marks: 56+19(Internal Assessment)**

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of EIGHT questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of eight short questions carrying 1 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 12 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**1. Photoinorganic chemistry**

**17Hrs**

Basics of photochemistry, Absorption, excitation, photochemical laws, quantum yield, electronically excited states, life times, measurements of the times, flash photolysis, energy dissipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, photochemical stages- primary and secondary processes, Kasha's rules, excited states, photosubstitution reactions, Adamson's rules, photo substitution reactions of Cr(III) and Ru(II) polypyridyles. Rh(III) ammine complexes. Ligand photoreactions, photoredox reactions, comparison of Fe<sup>2+</sup> and Ru<sup>2+</sup> complexes. Photo reactions and solar energy conversion, photosynthesis in plants and bacteriochlorophyll synthesis, photolysis of water using inorganic precursors.

**UNIT-II**

**2. Oxidative addition and Insertion reactions**

**15Hrs**

Acid base behavior of metal atom in complexes, protonation and Lewis base behavior, acceptor properties of Lewis acidity of complexes, oxidative and reductive elimination and their mechanism, addition of specific molecules, H<sub>2</sub>, HX and organic halide addition of some other molecules, reductive elimination, migration reactions their types, promotion of alkyl migration, insertion of CO into M-H bonds, other aspects of CO insertion reactions, transfer of other molecules, CO<sub>2</sub>, SO<sub>2</sub>, NO<sub>2</sub>, RCN.

### UNIT-III

#### 3. Transition metal compounds with hydrogen and oxad reactions 13Hrs

Insertion of alkenes and C-C unsaturated compounds, cleavage of C-H bonds, alkane activation. Cyclometallation reactions in detail, reactions of free hydrocarbons.

Characteristics of hydride complexes, synthetic methods, chemical behavior of H<sup>-</sup> complexes, mononuclear and homoleptic polyhydride anions, carbonyl H<sup>-</sup> and anion H<sub>2</sub> compounds, M-H interactions. Complexes of boron and aluminium hydrides, synthetic applications of metal hydrides.

### UNIT-IV

#### 4. Structure and bonding of d-Block elements 15Hrs

Pervoskite, Ti(NO<sub>3</sub>)<sub>4</sub>, TiCl<sub>4</sub>(diars)<sub>2</sub>, [Ti(OEt)<sub>4</sub>]<sub>4</sub>, Zr(BH<sub>4</sub>)<sub>4</sub>, [M<sub>6</sub>X<sub>12</sub>]<sup>+</sup> (M= Nb & Ta; X= halide); VO(acac)<sub>2</sub>; VOCl<sub>2</sub>(NMe<sub>3</sub>)<sub>2</sub>, [Nb(n<sup>5</sup>-C<sub>5</sub>H<sub>5</sub>)H-□ (n<sup>5</sup>, n<sup>1</sup>-C<sub>5</sub>H<sub>4</sub>)<sub>2</sub>]; Isopoly and heteropoly acids of MO, W & V; [M<sub>6</sub>X<sub>8</sub>]<sup>4+</sup> M= MO & W; CrO(O<sub>2</sub>) (bipy); [MO<sub>2</sub>O<sub>4</sub>(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub> (H<sub>2</sub>O)<sub>2</sub>]<sup>2+</sup>; [W<sub>3</sub>O<sub>2</sub> (O<sub>2</sub>CMe)<sub>6</sub> (H<sub>2</sub>O)<sub>3</sub>]<sup>2+</sup>; [Cr<sub>3</sub>O(O<sub>2</sub>CMe)<sub>6</sub> L<sub>3</sub>]<sup>+</sup>; [H<sub>2</sub>W<sub>2</sub>(CO)<sub>9</sub>]<sup>2+</sup>; Re<sub>3</sub>Cl<sub>9</sub>; [ReH<sub>9</sub>]<sup>3+</sup>; ReCl<sub>6</sub>(Pet<sub>3</sub>)<sub>2</sub>; Re<sub>2</sub>Cl<sub>6</sub>(PEt<sub>3</sub>)<sub>2</sub>; Re<sub>2</sub>Cl<sub>5</sub> (DTH)<sub>2</sub>, Roussin's salts; [Ir<sub>3</sub>O(SiO<sub>4</sub>)<sub>9</sub>]<sup>10-</sup>; [Ir<sub>3</sub>N(SiO<sub>4</sub>)<sub>6</sub>(H<sub>2</sub>O)<sub>3</sub>]<sup>4-</sup>; [Co(acac)<sub>2</sub>]<sub>4</sub>, α and β-MCl<sub>2</sub> (M=Pd, Pt); Wolfram's salt; [Ni(acac)<sub>2</sub>]<sub>3</sub>; Ni(Me<sub>6</sub>-acac)<sub>2</sub>; Ni (Me-sal)<sub>2</sub>; [Cren<sub>3</sub>] [Ni(CN)<sub>5</sub>] 1.5 H<sub>2</sub>O; [Ni (CN)<sub>2</sub> (NH<sub>3</sub>)]<sub>3</sub>. xC<sub>6</sub>H<sub>6</sub>; [Pd(O<sub>2</sub>CMe)<sub>2</sub>]<sub>3</sub>, [Pt(O<sub>2</sub>CMe)<sub>2</sub>]<sub>4</sub>; [PtMe<sub>3</sub>(acac)]<sub>2</sub>; helical chain of AuF<sub>3</sub>, Silver (III) ethylenedibiguanide ion; [CuXL]<sub>4</sub> X=halide, L = P or As Ligand; [Au<sub>3</sub>Cl<sub>2</sub>(PMe<sub>2</sub>Ph)<sub>10</sub>]<sup>3+</sup>; [Zn(acac)<sub>2</sub>]<sub>3</sub>; [Cd{S=C(NHCH<sub>3</sub>)<sub>2</sub>}<sub>2</sub>(SCN)<sub>2</sub>]; Hg(NH<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>

#### Books Recommended:

1. Chemistry of Elements by N. N. Greenwood and Earnshaw, Pergamon Press
2. W. W. Portfield: Inorganic Chemistry: A Unified approach
3. Cotton and Wilkinson: Advanced inorganic Chemistry: V<sup>th</sup> edition

*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester- IV)*  
**CH 425/MHCH 424: Organic Chemistry-VI**  
*Asymmetric synthesis, Green Chemistry and Heterocyclic Chemistry*

**60Hrs.**

**Time: 6 Hrs/week.**

**Max. Marks: 56+19(Internal Assessment)**

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of EIGHT questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
- III. Section-I will consist of eight short questions carrying 1 Mark each.
- IV. Section-II, III, IV and V of paper will consist of EIGHT questions in total having TWO questions from each unit of the syllabus and each question carry 12 Marks.
- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**1. Asymmetric Synthesis**

**(a) General Aspects**

**7Hrs**

Introduction, Analytical methods for determination of enantiomeric purity – GC, HPLC and NMR. Natural sources of chiral starting materials, classification and methods of formation of new chiral compounds.

**(b) Non-Enzymatic Approaches towards asymmetric synthesis**

**8Hrs**

Methods of asymmetric synthesis using chiral pool synthesis, auxiliaries, chiral reagents and catalysts, Asymmetric carbon-carbon bond formation using alkylation, Michael reaction and addition to carbonyl compounds. Cram's rule and Felkin-Ahn model. Asymmetric oxidation and reductions.

**UNIT-II**

**2. Enzymatic approach towards asymmetric synthesis**

**8Hrs**

Biotransformations: Nomenclature and Classification of enzymes, advantages and disadvantages, Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-menten and Lineweaver-Burk plots, reversible and irreversible inhibition. Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion.

**3. Reaction Catalysed by Enzymes**

**7Hrs**

Nucleophilic displacement on a phosphorus atom, multiple displacement reaction and the coupling of ATP cleavage to endergonic processes. Transfer of sulphates, addition

and elimination reactions, enolic intermediates in isomerization reactions, Enzyme catalyzed carboxylation and decarboxylation.

### UNIT-III

#### 4. Co-Enzyme Chemistry

6Hrs

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological function of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD<sup>+</sup>, NADP<sup>+</sup>, FMN, FAD, vitamin B<sub>12</sub>.

#### 5. Green Chemistry approach towards synthesis

9Hrs

Principles and concepts of Green Chemistry, atom economic and uneconomic reactions, source and minimizing techniques of waste from chemical industry, homogeneous and heterogeneous catalysis, phase transfer catalysis, biocatalysis and photocatalysis. Principles of ultrasound and microwave assisted organic synthesis. Reactions in ionic liquids and other environmentally benign solvents, Future Prospects.

### UNIT-IV

#### 6. Heterocyclic Synthesis

##### (a) Introduction

3Hrs

Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reaction.

##### (b) Small Ring Heterocycles

3Hrs

Three-membered and four-membered heterocyclic –synthesis and reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes

##### (c) Six-Membered Heterocycles with one Heteroatom

5Hrs

Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridones. Synthesis and reactions of quinolizinium and benzopyrylium salts, coumarins and chromones.

##### (d) Seven-and Large-Membered Heterocycles

4Hrs

Synthesis and reactions of azepines, oxepines, thiepinines, diazepines, thiazepines, azocines, diazocines, dioxocines and dithiocines.

#### Recommended Books:

1. Asymmetric Synthesis: The Essentials, Volume 1 Mathias Christmann, Stefan Bräse Wiley, 2008.
2. Principles of Biochemistry by Lehninger
3. Green Chemistry: An Introductory Text by Mike Lancaster, Royal Society of Chemistry, 2002
4. Principles of modern heterocyclic chemistry by Leo A. Paquette
5. Principles of Biochemistry By Voet and Voet

*M.Sc. Chemistry/M. Sc.(Hons.) Chemistry (Semester-IV)*  
**CH 426/MHCH 425: Physical Chemistry-V**  
*Surface and Polymer Chemistry*

**60 hrs.**

**Time: 6 Hrs/week.**

**Max. Marks: 56+19(Internal Assessment)**

**Instructions for paper setters and candidates**

- I. Examiner will make five sections of paper namely Section-I, II, III, IV and V
- II. Examiner will set total of EIGHT questions comprising ONE compulsory question of short answer type covering whole syllabi and TWO questions from each unit.
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- V. The students are required to attempt FIVE questions in all, taking ONE Compulsory question of section-I and one question from each section i.e. II, III, IV and V.

**UNIT-I**

**1. Adsorption**

**15Hrs**

Surface tension, capillary action, pressure difference across curved surface (Laplace equations), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electro-kinetic phenomena), catalytic activity at surfaces.

**UNIT-II**

**2. Micelles**

**15Hrs**

Surface active agents, classification of surface active agents, micellization, hydrophobic interactions, critical micellar concentration (CMC), factors affecting CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization, solubilization, micro emulsion, reverse micelles, applications of microemulsions.

**UNIT-III**

**3. Macromolecules**

**15Hrs**

**(a) Polymer** – definition, Different classifications of polymers, Linear, branched and network polymers. Basic concepts: monomers, repeat units, degree of polymerization. Types of polymers: electrically conducting polymers, Doping of polymers, mechanism of conduction, polarons and bipolarons, fire resistant, liquid crystal polymers, Molecular mass: number, mass and viscosity average weights; Molecular mass determination (osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, kinetics of polymerization, thermodynamics of polymerization. calculations of average dimensions of various chain structures. Importance of polymers,

Polymerization: condensation, addition, radical chain-ionic and co-ordination and copolymerization. Polymerization conditions and polymer reactions. Polymerization in homogenous and heterogeneous systems.

#### **UNIT-IV**

##### **(b) Structure and Properties:**

**15Hrs**

Polymer structure and properties-crystalline melting point  $T_m$ -melting point of homogenous series, effect of chain flexibility and steric factors, entropy and heat of fusion. The glass transition temperature,  $T_g$ -Relationship between  $T_m$  and  $T_g$ , effects of molecular weight, diluents, chemical structure, chain topology, branching and chain linking. Property requirements and polymer utilization.

##### **Books Suggested:**

1. Physical Chemistry, P. W. Atkins.
2. Textbook of polymer science, F. W. Billmeyer Jr. Wiley.
3. Polymer science, V. R. Gowariker, N. V. Viswanathan and J. Sreedhar, Wiley-Eastern.
4. Polymer Chemistry, Melcolm P. Stevens, Oxford University Press.
5. Physical chemistry of polymers, A. Tager, Mir Publisher, Moscow.