# **FACULTY OF SCIENCES**

### **SYLLABUS**

of

**Master of Science (Chemistry)** 

(Semester: I - IV)

(Under Continuous Evaluation System)

Session: 2021-22



# **The Heritage Institution**

# KANYA MAHA VIDYALAYA JALANDHAR (Autonomous)

### KANYA MAHA VIDYALAYA JALANDHAR (Autonomous)

#### SCHEME AND CURRICULUM OF EXAMINATION OF TWO YEAR DEGREE PROGRAMME

### Master of Science (Chemistry)

### (Session: 2021-22)

Master of Science (Chemistry)								
Semester I								
Course Code	Course Name	Course Type	Marks				Examination	
			Total	Ex		СА	<sup>_</sup> time (inHours)	
			I Utai	L	Р		(IIIIIours)	
MCHL-1081	Ligand Field Theory	С	50	40	-	10	3	
MCHL-1082	Organic Reaction Mechanism-I	С	50	40	-	10	3	
MCHL-1083	Physical Chemistry – Thermodynamics	С	50	40	-	10	3	
MCHL-1084	Spectroscopy A: Techniques for Structure Elucidation of Organic Compounds	С	75	60	-	15	3	
MCHM-1135	Computer for Chemists – Theory and Practical	С	75	40	20	15	3	
MCHP-1086	Inorganic Chemistry Practical(Quantitative Analysis)	С	75	-	60	15	3*2	
MCHP-1087	Organic Chemistry Practical	С	75	-	60	15	3*2	
	Total							

### KANYA MAHA VIDYALAYA JALANDHAR (Autonomous)

### SCHEME AND CURRICULUM OF EXAMINATION OF TWO YEAR DEGREE PROGRAMME

### Master of Science (Chemistry)

### (Session: 2021-22)

Master of Science (Chemistry) Semester II								
Total	Ext.		— CA	n time (inHours)				
MCHL-2081	Organometallics Chemistry	С	50	L 40	P -	10	3	
MCHL-2082	Organic Reaction Mechanism -II	С	50	40	-	10	3	
MCHL-2083	Physical Chemistry – Quantum Chemistry	С	50	40	-	10	3	
MCHL-2084	Reaction Mechanisms and Metal clusters	С	50	40	-	10	3	
MCHL-2085	Spectroscopy B: Techniques for Structure Elucidation of Inorganic Compounds	С	75	60	-	15	3	
MCHL-2336 MCHL-2057	Mathematics for Chemists	С	25	20		5	3	
	Biology for Chemists				-			
MCHP-2088	Organic Chemistry Practical	С	75	-	60	15	3*2	
MCHP-2089	Physical Chemistry Practical	С	75	-	60	15	3*2	
	Total		450					

### KANYA MAHA VIDYALAYA JALANDHAR (Autonomous)

### SCHEME AND CURRICULUM OF EXAMINATION OF TWO YEAR DEGREE PROGRAMME

### Master of Science (Chemistry)

### (Session: 2021-22)

Master of Science (Chemistry)								
Semester-III								
Course Code		Course Type	Marks				Examination	
			Total	Ext.		СА	time	
				L	Р		(in Hours)	
MCHL-3081	Inorganic Chemistry-II	С	50	40	-	10	3	
MCHL-3082	Organic Synthesis	С	50	40	-	10	3	
MCHL-3083	Surface and Polymer Chemistry	·C	50	40	-	10	3	
MCHL-3084	Electrochemistry and ChemicalDynamics	C	50	40	-	10	3	
MCHL-3085	Photochemistry and Pericyclic reactions	С	50	40	-	10	3	
MCHP-3086	Inorganic Chemistry Practical (Preparations)	Ċ	75	-	60	15	3*2	
MCHP-3087	Physical Chemistry Practical	C	75	-	60	15	3*2	
Total			400					

### SCHEME AND CURRICULUM OF EXAMINATION OF TWO YEAR DEGREE PROGRAMME

### Master of Science (Chemistry)

### (Session: 2021-22)

Master of Science (Chemistry) Semester IV								
Total	Ext.		СА	on time				
	L	Р		(in Hours)				
MCHL-4081	Advanced Inorganic Chemistry	С	75	60	-	15	3	
MCHL-4082	Chemistry of Natural Products	С	75	60	-	15	3	
MCHL-4083	Chemistry of Materials	С	75	60	-	15	3	
MCHP-4084	Advanced Practical- Organic Synthesis	С	50	-	40	10	3*2	
MCHP-4085	Advanced Practical- Inorganic Synthesis	С	50	-	40	10	3*2	
MCHP-4086	Advanced Practical- Physical Chemistry	С	50	-	40	10	3*2	
Total			375					

# Session 2021-22 COURSE CODE: MCHL-1081 Course Title: Ligand Field Theory (Theory)

#### **Course outcomes:**

Students will be able to

- CO1: illustrate an understanding of the principles of theories of metal-ligand bond.
- CO2:demonstrate an understanding of spectra of coordination compounds.
- CO3:analyze the spectra of transition metal ions.
- CO4: analyze Tanabe Sugano and Orgel diagrams.
- CO5: interpret the stability of complexes.
- CO6:understand the electronic spectra in transition metal complexes.
- CO7: learn mathematical rules for the formation of a group and Point groups
- CO8:construct the Character table for various point group and to determine the

symmetry of hybrid orbitals

## (Semester-I) Session: 2021-22 COURSE CODE: MCHL-1081 COURSE TITLE: Ligand field Theory (Theory)

Time: 3Hrs

Max. Marks: 50 (Theory: 40, CA: 10)

#### Note: The students are allowed to use Non-Programmable Calculator.

#### **Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

#### UNIT-I

#### **Symmetry**

Symmetry elements, symmetry operations and their matrix representation, group postulates and types, multiplication tables, point group determination, determination of reducible and irreducible representations, character tables, construction of character tables for  $C_{2v}$ ,  $C_{3v}$  (non-abelian group), use of symmetry in obtaining symmetry of orbitals in molecules, use of character table to determine which metal orbitals are used in  $\sigma$  and  $\pi$  bond formation in octahedral, tetrahedral and square planar transition metal complexes, qualitative splitting of s, p, d, f orbitals in octahedral, tetrahedral and square planar fields using character tables and without the use of charactertables.

#### **UNIT-II**

#### Molecular Orbital Theory for MetalComplexes:

Recapitulations, ligands symmetry orbitals and metal orbitals involved in molecular orbitals formation in octahedral complexes, MOEL diagrams for octahedral tetrahedral and square planar complexes showing  $\sigma$  and  $\pi$  bonding in transition metal complexes.

#### InterelectronicRepulsions:

Spin-spin, orbital-orbital and spin orbital coupling, LS and jj coupling schemes, determination of all the spectroscopic terms of  $p^n$ ,  $d^n$  ions, determination of the ground state terms for  $p^n$ ,  $d^n$ ,  $f^n$  ions using L.S. scheme, determination of total degeneracy of terms, order of interelectronic repulsions and crystal field strength in various fields, two type of electron repulsion parameters, spin orbit coupling parameters ( $\lambda$ ) energy separation between different j states, The effect of octahedral and tetrahedral fields on S, P, D and F terms (with help of the character table), splitting patterns of and G, H and Iterms

#### **UNIT-III**

#### Free Ions in Medium and Strong CrystalFields:

Strong field configurations, transition from weak to strong crystal fields, evaluation of strong crystal field terms of d<sup>2</sup> configuration in octahedral and tetrahedral crystal fields (using group theory), construction of the correlation energy level diagrams of d<sup>2</sup> configuration in octrahedral field, study of energy level diagrams for higher configurations, selection rules of electronic transitions in transition metal complexes, their proof using group theory, relaxation of the selection rule in centrosymmetric and non-centrosymmetric molecules, Orgel diagrams, Tanabe Sugano diagrams

#### **Magnetic Properties:**

Van Vlecks formula for susceptibility, first order Zeeman effect, second order Zeeman effect, KT states, quenching of orbitals angular momentum by ligand field, the magnetic properties of A and E terms, the magnetic properties of T terms, electronic delocalization, magnetic properties of  $d^n$  and  $f^h$  metal ions.

#### **UNIT-IV**

#### **Electronic Spectra of Transition MetalComplexes:**

Variation of the Racah parameter, nephlauxetic effect -central field covalency, symmetry restricted covalency, differential radial expansion, spectrochemical series, band intensities, factors influencing band widths, discussion of electronic spectra of octahedral and tetrahedral d<sup>1</sup> – d<sup>9</sup> metal ions, calculation of 10Dq and B with use of Orgel and Tanabe Sugano diagrams, low spin complexes of  $Mn^{3+}$ ,  $Mn^{2+}$ ,  $Fe^{3+}$ ,  $Co^{3+}$ ,  $Fe^{2+}$ , comment on the spectra of second and third transition series, spectra of K<sub>3</sub>MoCl<sub>6</sub> and [Rh(NH<sub>3</sub>)<sub>6</sub>]<sup>3+</sup>, spectra of cis and trans[Co(en)<sub>2</sub>X<sub>2</sub>]<sup>+</sup>, [Mn(H<sub>2</sub>O)<sub>6</sub>]<sup>2+</sup>, CuSO<sub>4</sub>.5H<sub>2</sub>O and its anhydrous complex, comparison of d–d band with f–f bands. Introduction to Charge Transfer Spectra.

- 1. F.A. Cotton, Chemical Application of Group Theory, WileyEastern.
- 2. G. L. Miessler, D. A. Tarr, Inorganic Chemistry, 3<sup>rd</sup> edition, PearsonEducation.
- 3. B.N. Figgis, Introduction to Ligand Field, Wiley Eastern.
- 4. A.B.P. Lever, Inorganic Electronic Spectroscopy, Elsevier.
- 5. A. Earnshaw, Introduction to Magnetochemistry, Academic Press.
- 6. J.E. Huheey, Inorganic Chemistry Principles of Structure and Reactivity, Harper Interscience.
- 7. R.S. Drago, Physical Method in Chemistry, W.B. SaundersCompany.
- 8. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, WileyInter-science.

# Master of Science (Chemistry) (Semester-I) Session: 2021-22 COURSE CODE: MCHL-1082

#### **COURSE TITLE: Organic Reaction Mechanism- I (Theory)**

#### **Course outcomes:**

Students will be able to

CO1:acquire the skills for correct stereochemical assignment and interpretation

in simple organic molecules.

CO2: formulate his/her own reasoned opinions in the mechanistic side of organic

Reactions

CO3: learn the concept of stereochemistry and its importance

CO3: understand the various types of aliphatic and aromatic nucleophilic substitution reaction and their mechanism

CO4:understand the concept and various types of aromaticity

CO5: know about the stereochemical problems in relation to chemical transformations

CO6:know synthetically the processes relevant organic-chemical reactions and be able

to discuss the mechanism of these reactions

# Master of Science (Chemistry) (Semester-I) Session: 2021-22 COURSE CODE: MCHL-1082 COURSE TITLE: Organic Reaction Mechanism- I (Theory)

**Time:3 Hrs** 

Max. Marks: 50

(Theory: 40, CA: 10)

#### Note: The students are allowed to use Non-Programmable Calculator.

#### **Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from anySection.

#### UNIT-I

#### Nature of Bonding in OrganicReactions:

Aromaticity in Benzenoid and non-benzenoid compounds. Huckel's Rule, Alternant and nonalternant hydrocarbons. Energy levels of  $\pi(pi)$  molecular orbitals in simple systems. Annulenes, Antiaromaticity, Homoaromaticity, PMO approach.

#### **Stereochemistry:**

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.

#### UNIT-II

#### **Reaction Mechanism, Structure and Reactivity:**

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, Kinetic and thermodynamic control in product formation. Transition states and reaction intermediates, Isotope effects, Hard and Soft Acid Base concept, Study of reactive intermediates – Types of intermediates, isolation and detection of intermediates (including use of spectral techniques), trapping of intermediates.

#### Aliphatic Nucleophilic Substitution –A:

The SN2, SN1and SNi mechanisms, mixed SN<sup>1</sup>& SN<sup>2</sup> mechanism SET mechanism. The neighbouring group mechanism (anchimeric assistance).Neighbouring group participation by pi and sigma bonds.

#### UNIT-III

#### Aliphatic Nucleophilic Substitution – B:

Classical, non-classical &phenonium cations, Rearrangements in carbocations (general survey).Ester hydrolysis.Nucleophilic substitution at allylic, aliphatic trigonal and vinylic carbon.Effect on the reactivity due to – substrate structure, attacking nucleophile, leaving group and reaction medium.Ambident nucleophiles and substrates, regioselectivity. Meyer's synthesis of aldehydes, ketones, acids and esters.Alkylation by organoboranes.

#### Aliphatic Electrophilic Substituion:

Bimolecular mechanism – SE2 and SEi. The SE1 mechanism, Hydrogen exchange, electrophilic substitution accompained by double bond shifts, diazo-transfer reaction, formation of sulphurylides, effect of substrates, leaving group and solvent polarity on the reactivity.

#### **UNIT-IV**

#### Aromatic Electrophilic Substitution:

The arenium ion mechanism, orientation and reactivity in mono substituted and di substituted aromatics. Energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems.Quantitative treatment of reactivity in substrates and electrophiles.Diazo coupling, Vilsmeir reaction, Gattermann-Koch reaction, Pechmann reaction, Houben – Hoesch reaction, Fries rearangement.

#### Aromatic Nucleophilic Substitution:

SNAr, SN1, benzyne and SRN1 mechanisms.Reactivity effect of substrate structure, leaving group and nucleophile.The von Richter, Sommelet-Hauser, and Smiles rearrangements.

- 1. Stereochemistry -Eliel
- 2. Advanced Organic Chemistry JerryMarch.
- 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 TextBook.
- 5. Stereochemistry conformation and Mechanism P. S.Kalsi

# Master of Science (Chemistry) (Semester-I) Session: 2021-22 COURSE CODE: MCHL-1083 COURSE TITLE: Physical Chemistry – Thermodynamics (Theory)

#### **Course outcomes:**

Students will be able to

CO1: calculate change in thermodynamic properties, equilibrium constants, partial molar quantities, chemical potential. Identify factors affecting equilibrium constant.

CO2: apply phase rule and, draw phase diagrams for one, and two component systems, identify the dependency of temperature and pressure on phase transitions, and identify first/second order phase transitions.

CO3: solve problems based on Debye-Huckel limiting law, calculate excess thermodynamic properties.

CO4: calculate the absolute value of thermodynamic quantities (U, H, S, A, G) and equilibrium constant (K) from spectroscopic data.

CO5: predict heat capacity ( $C_v$ ,  $C_p$ ) of an ideal gas of linear and non-linear molecules from the number of degrees of freedom, rotational and vibrational wave numbers.

CO6: derive the temperature dependence of the second Virial coefficient (real gases) from interatomic potentials.

CO7: explain T<sup>3</sup> dependence of heat capacity of solids at low temperatures (universal feature) using Debye and Einstein theory of heat capacity of solids.

CO8: explain the concept of Fermi energy in metals and use it to calculate the chemical potential of conduction.

#### Master of Science (Chemistry)

#### (Semester-I)

#### Session: 2021-22

#### **COURSE CODE: MCHL-1083**

#### **COURSE TITLE: Physical Chemistry – Thermodynamics**

(Theory)

Time: 3 Hrs.

Max. Marks: 50

(Theory: 40, CA: 10)

# Note: The students are allowed to use Non-Programmable Calculator. Instructions for the Paper Setters:

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

#### UNIT-I

#### **Classical Thermodynamics**

Brief resume of concepts of thermodynamics, 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

#### 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. Application of phase rule to three component system, second order phase transitions.

#### **Statistical Thermodynamics:**

Concept of distribution law, thermodynamic probability and most probable distribution, Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and micro canonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers).

#### UNIT-III Partition functions

Translational, rotational, vibrational and electronic partition function, calculation of thermodynamic properties in terms of partition functions. Application of partition functions.

Heat capacity behavior of solids-chemical equilibria and equilibrium constants in terms of partition functions, Fermi-Dirac statistics, distribution laws, and application to metals. Bose-

Einstein statistics- distribution law and application to helium.

#### UNIT-IV

#### Non Equilibrium Thermodynamics:

Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of generalized fluxes and forces, non-equilibrium stationery states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electro kinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

- 1. I F Nash: Elements of classical and statistical thermodynamics
- 2. Lee Bot: Irreversible thermodynamics
- 3. Thermodynamics of Biological Processes, D. Jou and J.E. LeeBot
- 4. I Prigogine: Introduction to thermodynamics of irreversible processes
- 5. T L Hill: Introduction to statistical thermodynamics.

### Master of Science (Chemistry) (Semester-I) Session: 2021-22 COURSE CODE: MCHL-1084 COURSE TITLE: SPECTROSCOPY – A: Techniques in Structure Elucidation of Organic Compounds (Theory)

#### **Course outcomes:**

Students will be able to

CO1:learn about the Principle and applications of ultraviolet and Woodward Fisher Rule

CO2: understand the infra-red spectroscopy in organic structure determination

CO3:know about the Nuclear magnetic resonance spectroscopy. Proton chemical shift,

spin-spin coupling, coupling constants and applications to organic structures <sup>13</sup>Cresonance spectroscopy

CO4:learn the Mass spectrometry and its applications

CO5: to know about the Vibrational spectroscopy, Vibrational coupling overtones and Fermi resonance.

CO6: apply NMR, IR, MS, UV-Vis spectroscopic techniques in solving structure of organic molecules and in determination of their stereochemistry.

CO7: interpret the above spectroscopic data of unknown compounds.

CO8:use these spectroscopic techniques in their research.

#### Master of Science (Chemistry)

(Semester-I)

#### Session: 2021-22

#### **COURSE CODE: MCHL-1084**

### **COURSE TITLE: SPECTROSCOPY – A: Techniques in Structure Elucidation of Organic**

#### Compounds

(Theory)

Max. Marks: 75

Time: 3 Hrs.

(Theory: 60, CA:15)

# Note: The students are allowed to use Non-Programmable Calculator. Instructions for the Paper Setters:

Eight questions of equal marks (twelve each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITS I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from anySection.

#### UNIT-I

#### Nuclear MagneticResonance

The Nuclear spin, Larmor frequency, the NMR isotopes, population of nuclear spin level, spin and spin lattice relaxation. Measurement techniques (CW & FT method), solvent used. Chemical shift, reference compounds, shielding constant, range of typical chemical Shifts simple application of chemical shifts, ring current and aromaticity.Shifts for <sup>1</sup>H and <sup>13</sup>C. - Spin-spin interactions, Low and High resolution spectra with various examples, Correlation of H bound to carbon, H bound to other nuclei such as nitrogen, oxygen, sulphur, Complex spin-spin interaction, between two or more nuclei. Effect of chemical exchange, fluxional molecules, Hindered rotation on NMR spectrum Karplus relationship, nuclear magnetic double resonance, chemically induced dynamic nuclear polarization. Brief introduction to multipulse NMR spectroscopy, Application of structure elucidation of simple organic molecules Lanthanide shift.

#### **UNIT-II**

#### MassSpectroscopy

Elementary theory - Measurement techniques (EI, CI, FD, FAB), Resolution, exact masses of nuclides, Molecular ions, isotope ions, fragment ions of odd and even electron types, rearrangement ions, Factors affecting cleavage patterns, simple cleavage, cleavages at a hetero atom, multicentre fragmentations rearrangements, Reteroiels – Alder fragmentation. Cleavage associated with common functional groups (Aldehydes, ketones cyclic and acyclic esters, alcohols, olefins, aromatic compounds amines). - Special methods of GCMS, high resolution MS, Introduction to radical anion mass spectroscopy. Interpretation of the spectrum of an unknown.

#### Ultraviolet and VisibleSpectroscopy

The energy of electronic excitation, measurement techniques, Beer-Lambert Law, Molar extinction coefficient. The Frank Condon Principle. Different types of transition noticed in UV spectrum of organic functional groups and their relative energies. Chromophore, auxochromes, factors affecting max, Effect of steric hindrance to coplanarity, Solvent Effects. Applications of U.V. spectroscopy.

#### UNIT-III

#### InfraredSpectroscopy

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 reactionkinetics.
- (c) Determining purity and quantitative analysis.
- (d) Studying hydrogenbonding.
- (e) Studying molecular geometry & conformationalanalysis.
- (f) Studying reactivespecies

#### **UNIT-IV**

- 1. Solution of Structural Problems by Combined Use of the following Spectroscopic Techniques:
- (a) Electronicspectra
- (b) Vibrational spectroscopy
- (c) NMR (<sup>1</sup>H and <sup>13</sup>C) spectroscopy
- (d) Mass Spectroscopy

- 1. W. Kemp. OrganicSpectroscopy.
- 2. W. Kemp. N.M.R.Spectroscopy.
- 3. D.H. Williams and I. Fleming. Spectroscopic Methods in OrganicChemistry.
- 4. R.M. Silverstein & G.C. Bassler, Spectrometric Identification of OrganicCompounds.
- 5. Introduction to Spectroscopy Pavia

## Master of Science (Chemistry) (Semester-I) Session: 2021-22 COURSE CODE: MCHM-1135 COURSE TITLE: Computer for Chemists

#### **Course outcomes:**

At the end of the course, the learners should be able to:

CO1: write short simple programs in C language and be able to compile and execute them in a host of machines.

CO2: use standard software tools to perform algebraic and numerical calculations often required in elementary physical chemistry in the areas of quantum chemistry, spectroscopy, kinetics and thermodynamics

Master of Science (Chemistry) (Semester-I) Session: 2021-22

### COURSE CODE:MCHM-1135 COURSE TITLE: Computer for Chemists

Total Marks: 75 (Theory: 40, CA:15) Practical Marks: 20

#### Note: The students are allowed to use Non-Programmable Calculator.

#### **Instructions for the Paper Setters:**

**Time:**(3+3) Hrs.

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from anySection.

#### 1. Computer Programming in Clanguage

#### 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.

#### UNIT-II

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

Decision making in C, scanf function, relational operators, logical operators, if statement, if else statement, nesting of if statement.

#### UNIT-III

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.

#### UNIT-IV

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.

#### 2. Computer programs inChemistry

#### (these are also be done in the practical class):

Development of small computer codes involving simple formulae in chemistry:

#### UNIT-I

- 1. Calculation of mean, median, mode.
- 2. Solution of a quadratic equation.
- 3. Calculation of linearregression.
- 4. Calculation of curve linearregression.

#### UNIT-II

- 5. Calculation of Bohr orbit from de Broglie Lambda forelectron.
- 6. Calculation of wave number and frequency from value of wavelength.
- 7. Calculation of van der Waalsradii.
- 8. Radioactivedecay.
- 9. Rate constant of a 1st order reaction, 2nd orderreaction.
- 10. Calculation of lattice energy using Born Landeequation.

#### **UNIT-III**

- 11. Addition, multiplication and solution of inverse of 3 X 3matrix.
- 12. Calculation of average molecular weight of a polymer containing n1 molecules of molecular weight m1, n2 molecules of molecular weight m2 and soon.
- 13. Program for calculation of molecular weight of organic compound containing C, H, N, O and S.
- 14. Calculation of reduced mass of diatomicmolecule.
- 15. Calculate the RMS and most probable velocity of agas.

#### **UNIT-IV**

- 16. Calculate the ionic mobility from ionic conductancevalues.
- 17. Determine the thermodynamic parameters for isothermal expansion of monoatomic idealgas.
- 18. Calculation of value of g- factor from value of J andS.
- 19. Calculate the bond length and bond angles using crystal structuredata.

- 1. K.V. Raman, Computers in Chemistry, Tata McGraw Hill.
- 2. Mullish Cooper, The spirit of c, An Introduction to ModernProgramming.

# Master of Science (Chemistry) (Semester-I) Session: 2021-22 COURSE CODE:MCHP-1086 COURSE TITLE: INORGANIC CHEMISTY (PRACTICAL) (Quantitative Analysis)

#### **Course outcomes:**

Students will be able to

CO1:determine the strength of ions by Oxidation reduction titrations

CO2: estimate the amount of ions by precipitation titrations

CO3:estimate the amount of ions by complexometric and gravimetric methods

#### Master of Science (Chemistry)

#### (Semester-I)

#### Session: 2021-22

#### **COURSE CODE: MCHP-1086**

#### **COURSE TITLE: INORGANIC CHEMISTY (PRACTICAL)**

#### (Quantitative Analysis)

Time: 6 Hrs.

#### Max. Marks: 75

#### (P: 60, CA: 15)

**Instruction for practical examiner:** Question paper is to be set on the spot jointly by the Internal and External Examiners. Two copies of the same should be submitted for the record to COE Office, Kanya Maha Vidyalaya, Jalandhar.

#### I. Oxidation-ReductionTitrations

- 1. Standardization with sodium oxalate of  $KMnO_4$  and determination of  $Ca^{2+}ion$ .
- 2. Standardization of ceric sulphate with Mohr's salt and determination of  $NO_3^{-1}$  and  $C_2O_4^{-2}$  ions.
- 3. Standardization of  $K_2Cr_2O_7$  with  $Fe^{2+}$  and determination of  $Fe^{3+}$  (Ferricalum)
- Standardization of hypo solution with potassium iodate / K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> and determination of available Cl<sub>2</sub> in bleaching powder, Sb<sup>3+</sup> andCu<sup>2+</sup>.
- 5. Determination of hydrazine with KIO<sub>3</sub>titration.

#### **II. Precipitation Titrations**

- 1. AgNO<sub>3</sub> standardization by Mohr's method by using adsorptionindicator.
- 2. Volhard's method for Cl<sup>-</sup>determination.
- 3. Determination of ammonium / potassiumthiocyanate.

#### **III.** ComplexometricTitrations

- 1. Determination of  $Mg^{2+}$  and  $Mn^{2+}$  in a mixture using fluoride ion as a demaskingagent.
- 2. Determination of Ni<sup>2+</sup> (backtitration).
- 3. Determination of  $Ca^{2+}$  (by substitutionmethod).

#### **IV. GravimetricAnalysis**

- 1. Determination of  $Ba^{2+}$  as its chromate.
- 2. Estimation of lead as its leadmolybdate.
- 3. Estimation of chromium (III) as its leadchromate.
- 4. Estimation of Cu<sup>2+</sup> using Ammonium/ Sodiumthiocyanate.

#### **Books Recommended:**

Vogel's book on Inorganic Quantitative Analysis

## Master of Science (Chemistry) (Semester I) Session: 2021-22 COURSE CODE: MCHP-1087 COURSE TITLE: ORGANIC CHEMISTRY (PRACTICAL)

#### **Course outcomes:**

The students will be able to

- CO1:independently perform two step organic synthesis.
- CO2: identify the synthesized compounds by TLC
- CO3:perform analysis of common analgesic drugs by TLC
- CO4:extract, identify and characterize the compounds isolated from naturalproducts

#### Master of Science (Chemistry) (Semester I) Session: 2021-22 COURSE CODE:MCHP-1087 COURSE TITLE: ORGANIC CHEMISTRY (PRACTICAL)

#### Time: 6Hrs.

Max. Marks: 75 (P: 60, CA: 15)

**Instruction for practical examiner:** Question paper is to be set on the spot jointly by the Internal and External Examiners. Two copies of the same should be submitted for the record to COE Office, Kanya Maha Vidyalaya, Jalandhar.

#### UNIT-I

- 1. **Purification and Characterization of Organic Compounds**, the student is expected to carry out the experiments of purification (fractional crystallization, fractional distillation, chromatography) separation, purification and identification of the compounds of binary organic mixture (liquid-liquid, liquid-solid and solid-solid), using chemical analysis and IR and PMR spectral data. The student should also check the purity of the separated components on TLCplates.
- 2. To carry out the analysis of common analgesic drugs by thin layer chromatography, Acetaminophen, Aspirin, caffeine, phenacetin, salicylamide. (Learn to check purity of the given samples and completion of the chemical reactions).

#### UNIT-2

**Organic Synthesis and Extraction of Organic Compounds from Natural Sources**. The student is expected to carry out 4 to 6 organic preparations (usually involving not more than two steps), some of the illustrative experiments are listed below:-

1. Extraction of Caffeine from tealeaves

(Ref. Experiment Organic Chemistry, (H. Dupont Durst, George W. Gokel, P 464 McGraw Hill Book Co., New York).

Student would be asked to purity crude sample, check the purity on a TLC single spot and get the NMR scanned and interpret (Three methyl singlets and I methane singlet).

- 2. Isolation of casein from milk (try some typical colour reactionsproteins).
- 3. *Synthesis of 2-phenyllndole-Fischer Indole Synthesis*. Book 1, p.852 **Aim:** To Study condensation and cyclization reactions.
- 4. Synthesis of 3-nitrobenzoic from benzoic acid (Rf. Ibid., p.245-247 and 443-448). Aim: To demonstrate the process of meta nitration, esterification and saponification of an ester. Make a comparative study of IR and PMR spectra of benzoic acid, methyl benzoate, methyl3-nitrobenzoate.
- 5. *Cannizaro's reaction of 4-chlorobenzaldehyde*.. Book 1, p760 Aim: To demonstrate technique of isolation of two products from the reaction mixture and the procedure of intermolecular hydride transfer. Make a comparative study of IR and PMR spectra of 4 chlorobenzadehyde, 4-chlorobenzoic acid 4-chlorobenzyl alcohol.
- 6. *Synthesis of 1,3,5-Tribromobenzene from aniline*. Aim: To demonstrate: Bromination, Diazotization andReduction.

#### **Books Recommended:**

Vogel's Text book of practical organic chemistry, 5<sup>th</sup> edition.

### Master of Science (Chemistry) (Semester-II) Session: 2021-22 COURSE CODE: MCHL-2081 COURSE TITLE: ORGANOMETALLICS CHEMISTRY (Theory)

#### **Course outcomes:**

Students will be able to

CO1: familiarize with the organometallic reaction mechanisms and its applications

CO2: learn about the Catalysis, hydrogenation of olefins and Oxo process

CO2: study the concept of oxidation of olefins and polymerization

CO3: demonstrate basic principles of organometallic compounds.

CO4: illustrate stability of organometallic compounds.

CO5: identify the structure and bonding aspects of simple organometallic compounds

CO6:applydifferent electron counting rules to predict the shape/geometry of low and high nuclearity metal carbonyl clusters

CO7: identify different types of organometallic reactions and apply the above concepts to explain different catalytic reactions

CO8: familiarize with the reactions with and of coordination ligands

CO9:understand the role of pi acid ligands

# Master of Science (Chemistry) (Semester-II) Session: 2021-22 COURSE CODE: MCHL-2081 COURSE TITLE: ORGANOMETALLICS CHEMISTRY (Theory)

Time:3 Hrs.

Max. Marks: 50

(Theory: 40, CA: 10)

#### Note: The students are allowed to use Non-Programmable Calculator.

#### **Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from anySection.

#### UNIT-I Organometallics

Energy polarity and reactivity of M-C bond, Stability of Main group organometallics: Methods of preparation in perspective-organolithium compounds: structure and bonding & reaction-carbolithiatic organometallics of group 2 and 12 e.g. Mg and Zn, Cd and Hg: Preparation and structure of organoaluminium compounds, Technical applications of Tris (alkyl)aluminium compounds.  $\eta^2$ - ligands: olefenic and acetylenic complexes, chelating olefenic ligands – synthesis and structure.  $\eta^2$  – ligands: Allylic and  $\eta^4$  – complexes of cyclopentadiene.

#### UNIT-II

Synthesis and structure.  $\eta^4$  –ligands: Butadiene, cyclobutadiene, heterocyclic pentadiene (S, Se, Te). Classification, Nomenclature of cyclopentdienyl complex.MO treatment of ferrocene.  $\eta^6$  – ligands: Benzene and its derivatives. Multideckersandwichcompounds.

#### UNIT-III

Homogeneous hydrogenation of unsaturated compounds, reversible cis-dihydrocatalysis, monohydrido compounds, asymmetrical hydrogenation, hydrosilation of unsaturated compounds, hydrocyanation of alkenes, alkane metathesis, Ziegler-Natta polymerization of ethylene and propylene, water gas shift reaction, acetic acid synthesis by carbonyls, Oxopalladation reactions. Organometallic Reagents in Organic synthesis.

#### **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**

#### p-acid ligands

pi-acceptor character of CO, O<sub>2</sub>, N<sub>2</sub>, NO, PH<sub>3</sub> molecules in terms of MOEL diagram, Metal carbonyls; structure and bonding; vibration spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiaryphosphine as ligand.

- C. Elschenbroich and A. Salzer, Organometallics: A Concise Introduction, 2<sup>nd</sup>Ed., VCH 1992.
- 2. J.E. Huheey, Inorganic Chemistry Principles of Structure and Reactivity, Harper Interscience.
- F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Ed. V &VI.Wiley Interscience.
- 4. G. L. Miessler, D. A. Tarr, Inorganic Chemistry, 3<sup>rd</sup> edition, PearsonEducation

# Master of Science (Chemistry) (Semester-II) Session: 2021-22 COURSE CODE: MCHL-2082 COURSE TITLE: Organic Reaction Mechanism – II (Theory)

#### **Course outcomes:**

Students will be able to

CO1:learn about the addition reactions between a hetero atom and double bonded carbon

compounds

CO2: obtain an outline about elimination reactions and rules used to study elimination

reactions

CO3:learn about some specific examples of elimination reactions

CO4:learn the basic mechanism of oxidation in organic compounds

CO5:acquire knowledge about the reagents which causes oxidation and reduction in various compounds

CO6:learn about the formation of carbon - carbon bonds

Master of Science (Chemistry) (Semester-II) Session: 2021-22 COURSE CODE: MCHL-2082

**COURSE TITLE: Organic Reaction Mechanism – II (Theory)** 

Time: 3 Hrs.

Max. Marks: 50

(Theory: 40, CA: 10)

#### **Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from anySection.

UNIT-I

#### **1.Free Radical Reactions**

Types of free radial 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.Effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction, Free radical rearrangement, Hunsdiecker reaction, Kolbe reaction, Hydroxylation of aromatics by Fenton's reagent.

#### **2** Elimination Reactions

The E2, E1, E1cB mechanisms. Orientation of the double bond.Effects of substrate structure, attacking base, leaving group and medium on reactivity. Mechanism and orientation in pyrolytic eliminations.

#### UNIT-II

#### 3. Addition to Carbon – Carbon MultipleBonds

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydroboration, Michael reaction. Sharpless asymmetric epoxidation, Hydrogenation of double and triple bonds. Hydrogenation of aromatic rings.

#### 4. Addition to Carbon – Hetero Multiple Bonds –A

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles, Wittig reaction.

#### 5. Addition to Carbon – Hetero Multiple Bonds –B

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

#### 6. Formation of Carbon-Carbon Bond

Principle, disconnections and synthons, electrophilic and nucleophilic carbon species. Basecatalyzed condensations; Aldol condensation, Claisen reaction, Perkin reaction, Stobbe condensation, Darzen condensation, Knoevengal reaction, Use of malonic, acetoacetic and cyanoacetic esters, Micheal addition, Wittig reactions. Use of acetylides, Acid-catalyzed condensation – self condensation of olefins, Friedal-Craft's reactions, Fries reactions, Mannich reaction, Mannich bases as intermediates in organic synthesis. Four centrereactions. Diels-Alder reaction, 1-3 Dipolaradditions.

#### UNIT-IV

#### 7. Oxidation

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 tetraoxide, iodobenzene diacetate and thallium(III) nitrate.

#### 8. Reduction

Introduction .Different reductive processes. Hydrocarbons - alkanes, alkenes, alkynes and aromatic rings. Carbonyl compounds – aldehydes, ketones, acids and their derivatives. Epoxides.Nitro, nitroso, azo and oxime groups.Hydrogenolysis.

- 1. Principles of Organic Synthesis Norman and Coxon
- 2. Advanced Organic Chemistry JerryMarch.
- 3. Advanced Organic Chemistry, F.A. Carey, R.J.Sunberg.
- 4. Highlights of Organic Chemistry, W, J.L. Nobel; An Advanced TextBook.
- 5.Hand Book of Reagents for Organic Synthesis Oxidizing and Reducing Reagents. S. D. Burke and R. L. Danheiser (John Wiley and Sons)
- 6. Organic Synthetic reactions by WilliamCarruthers

#### Session: 2021-22

#### **COURSE CODE: MCHL-2083**

#### **COURSE TITLE: Physical Chemistry-Quantum Chemistry (Theory)**

#### **Course outcomes:**

Students will be able to

CO1: have basic idea about quantum chemistry and the mathematics associated with quantum statistics including certain aspects of linear algebra

CO2: apply this knowledge to atomic and molecular structure

CO3:usemathematical techniques in linear algebra for eigen values and eigen vectors and first and second order differential equations not only in quantum chemistry but in other areas of chemistry

CO4:solveall the model problems in quantum mechanics for which exact analytical methods and solutions are available and will apply them to analyze the basis behind the postulatory method of quantum mechanics and which forms the foundations for advanced study of the subject.

CO5:relateconcepts that were originally introduced purely as modern atomic physics to molecular systems through harmonic oscillator, spin and rigid rotator

### Session: 2021-22 COURSE CODE:MCHL-2083 COURSE TITLE: Physical Chemistry – Quantum Chemistry (Theory)

Time: 3 Hrs.

Max. Marks: 50

(Theory: 40, CA: 10)

#### Note: The students are allowed to use Non-Programmable Calculator.

#### **Instructions for the PaperSetters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from anySection.

#### UNIT-I

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

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.** 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 quantummechanics.

#### UNIT-III

#### 3. Applications of QuantumPostulates

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

#### 4. Angular Momentum

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 method for angular momentum, spin angular momentum and their relations

#### UNIT-IV

#### 5. General Orbital Theory of Conjugated Systems

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 cyclopropenylsystem.

#### 6. The ApproximateMethods

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

#### **Books Suggested:**

- 1. Physical Chemistry, A Molecular Approach by MacQuarrieandSimon.
- 2. Quantum Chemistry, Ira N. Levine, PrenticeHall.
- 3. Quantum Chemistry, H. Eyring, Kimball and Walter.
- 4. Quantum Chemistry, Atkin.
- 5. Fundamentals of Quantum Chemistry, Anantharaman.R.

## Master of Science (Chemistry)(Semester-II) Session: 2021-22 COURSE CODE: MCHL-2084 COURSE TITLE: REACTION MECHANISMS AND METAL CLUSTERS (Theory)

#### **Course outcomes:**

Students will be able to

CO1:describe the stability of metal complexes by the use of formation constants

and calculate thermodynamic parameters from them

CO2:learn the mechanism of substitution reaction and explain the parameters that affects the crystal structure of a compound

CO3:determine binary formation constants by different methods

CO4:understand the chemistry of inorganic rings , chains and metal clusters

#### Master of Science (Chemistry) (Semester-II) Session: 2021-22 COURSE CODE: MCHL-2084

#### COURSE TITLE: REACTION MECHANISMS AND METAL CLUSTERS (Theory)

Time:3 Hrs.

Max. Marks: 50

(Theory: 40, CA: 10)

#### Note: The students are allowed to use Non-ProgrammableCalculator.

#### **Instructions for the PaperSetters:**

Eight questions of equal marks (eight marks) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from anySection.

#### UNIT-I

#### **Reaction Mechanism of Transition Metal Complexes**

Inert and labile complexes, mechanisms of substitution (dissociative, associative interchange mechanism, the conjugate mechanism, substitution in *trans* complexes, substitution in *cis* complexes, isomerism of chelate rings), *trans* effect, explanation for *trans* effect, Ligand replacement reactions of square planar and octahedral complexes: their factors and mechanism of substitution, orbital occupation mechanisms. Anation reaction, Metal carbonyl reactions species with 17 electrons.

#### UNIT-II

Electron transfer processes with mechanism, key ideas concerning electron transfer reactions between transition Metals. Cross reactions and thermodynamics. Marcus theory, its kinetics and applications.

#### UNIT-III

Doubly bridged inner sphere transfer and other electron transfer reactions. Two electron transfer, non-complementary reactions. Stereochemical nonrigidity of coordinate and orgonometallic compounds, trigonal bypyramid, system with six or more coordination number. Isomerization and recemization of trischelates, metal carbonylscrambling.

#### Metal-ligand Equilibria in Solution

Stepwise and overall formation constant and their interaction, trends in step wise constant, factors affecting the stability of metal complex with reference to the nature of metal ion and ligand chelate effect and its thermodynamic origin. Determination of binary formation constants

by pH-meter, Job's method and spectrophotometery.

#### UNIT-IV

#### Inorganic Rings, Chains and Metal Cluster

Borazines, Phosphazenes and other heterocyclic inorganic ring, systems, homocyclic inorganic systems, cages of P and S, oxides &sulphides, Higher boranes and carboranes, methods of classifying boranes, Molecular orbit view of chlorohydroborane ions and carboranesmetallocarboranes, isopoly and heteropoly acids and salts; metal-metal bonds and bi-, tri-, tetra-, penta-, and hexanuclear clusters, electron counting schemes for HNCC's. Approaches to systematic cluster synthesis; mention of seven, eight and nine atom clusters. Isolobal analogy and examples of application of analogy.

- 1. K.P. Purcell and J. V. Kotz: Inorganic Chemistry W.B. Saunders Co. London,(1977).
- 2. G. L. Miessler, D. A. Tarr, Inorganic Chemistry, 3<sup>rd</sup> edition, PearsonEducation.
- 3. F.A. Cotton & Wilkinson: Inorganic Chemistry V & VI Ed. Willy Eastern –(1999).
- 4. J.E. Huheey: Inorganic Chemistry III & IV Ed. Pearson Education Asia -(2002).

#### Master of Science (Chemistry)(Semester-II)

#### Session: 2021-22

#### **COURSE CODE: MCHL-2085**

## COURSE TITLE: SPECTROSCOPY – B: Techniques for Structure Elucidation of Inorganic Compounds (Theory)

#### **Course outcomes:**

Students will be able to

CO1: identify symmetry elements and symmetry operations

CO2: determine the rotational spectra of linear molecules

CO3: determine IR and Raman activity of linear molecules

CO4: studyselection rules for electronic transitions

CO5: understand the principle and spectra interpretation of photoelectron spectroscopy, electron spin resonance spectroscopy, nuclear quadrupole resonance spectroscopy, Mossbauer spectroscopy

## Master of Science (Chemistry) (Semester-II) Session: 2021-22 COURSE CODE: MCHL-2085 COURSE TITLE: SPECTROSCOPY – B: Techniques for Structure Elucidation of Inorganic Compounds (Theory)

Time:3 Hrs.

Max. Marks: 75

(Theory: 60, CA:15)

# Note: The students are allowed to use Non-ProgrammableCalculator. Instructions for the PaperSetters:

Eight questions of equal marks (twelve each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITS I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

## UNIT – I Symmetry and Point Groups:

Definition of symmetry, symmetry elements, determination of point groups, introduction to use of character table in determining irreducible representation and symmetry of the atomic orbitals.

## UNIT – II

## Vibration and Rotation Spectroscopy: Infrared, Raman and Microwave

- Harmonic and Anharmonic oscillators, vibrational energies of diatomic molecules. Potential energy function for a chemical bond. Absorption of radiations by molecular vibration. Selection rules, forceconstant.

- Rotational energies of linear molecules. Rotational energy level populations, merits and demerits of microwave spectroscopy, rotational spectra of rigid, linear molecules, non-rigid rotators. Determination of moment of inertia and bond length from rotational spectra, relative intensities of spectral lines. Rotational spectra of non-linear molecules (brief mention), vibrations in polyatomic molecules. Effects giving rise to absorption bonds. Group vibrations and limitations of group vibrationconcepts.

- Polarisations of light. Theories of Raman Effect, Merits and demerits of Raman spectroscopy. Pure rotational Raman spectra of linear molecules. Vibrational Raman spectra selection rules. Rule of mutual exclusion. Rotational Fine IR spectra, vibroniccoupling.

- Sample handling. Factors affecting absorption frequencies. Interpretation and finger printing

- regions. Use of symmetry considerations to determine the number of active I.R, and

- Ramanlines (character tables to be provided in theExamination)

## UNIT-III

## (A)Applications

- of Raman and IR selection rules to the determination of Inorganic structure with special

- emphasis on:

(i) Metalcarbonyls. (ii)NSF<sub>3</sub> (iii) Geometrical isomerisan – differentiation between Cis and trans.  $[Co(bipy)_2Cl_2]Cl$ . (iv) Structures of CO<sub>2</sub>, N<sub>2</sub>O, H<sub>2</sub>O, chlorocomplexes of mercury, camium and zinc and some octahedral complexes ML<sub>6</sub> (eg. SiF<sub>6</sub><sup>2-</sup>, PF<sub>5</sub>,SF<sub>6</sub>). (v) Changes in the spectra of donor molecules upon coordination with special emphasis on N, N – dimethyl – acetamide and DMSO with Fe<sup>3+</sup>, Cr<sup>3+</sup>, Zu<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>.

## (B)Photo Electron Spectroscopy

Introduction, excitation & ejection of electrons, electronic energy levels in atoms and molecules, Core level photoelectron spectroscopy, symmetry & molecular orbitals, valence electron photo electron spectroscopy, valence excitation spectroscopy. Dissociation, Predissociation, change of shape on excitation.

## (C)Electron Spin Resonance Spectroscopy

Features of ESR spectra, measurement technique hyperfine coupling in isotropic system ( $C_5H_5$ ,  $C_6H_6$ ,  $C_{14}H_{10}$ , biphenyl) Anisotropic splitting, Electron – electron interaction, Transition metal complexes g-value and factors affecting g-value, zerofield splitting, Kramer's degeneracy, Rate of electron exchange, Application to p – benzoseniquinone DPPH, pyrazine. Double resonance technique ENDOR, ELDOR.

## UNIT – IV

## Nuclear Quadrupole Resonance Spectroscopy

Introduction, effects of magnetic field on the spectra. Relationship between the electric field gradient and molecular structure. Interpretation of eQ, data, the effect of crystal lattice on the magnitude of eQ4, double resonance technique, Application (PFCI<sub>4</sub>.PCI<sub>5</sub>), (NH<sub>4</sub>)<sub>2</sub>TeCl<sub>6</sub>, , group 14 tetra halides, R<sub>3</sub>MX<sub>2</sub> (M=As,Sb,Bi), Cis & Trans[Co(en)<sub>2</sub>Cl<sub>2</sub>]Cl, Polyhalide ion, BrCN, HIO<sub>3</sub> (1,2)

## **Mossbauer Spectroscopy**

Introduction, principles, conditions of MB spectra, parameters from MB spectra. Isomer shift electric quadrupole interaction, magnetic interaction, use of additive partial quadrupole splittings to predict quadrupole coupling. Application of  $\{{}^{57}F_{e}, {}^{119}S_{N}, {}^{151}E_{U}$  compounds, to biological systems to surface study, I<sub>2</sub>CI<sub>6</sub>, IBr<sub>2</sub> CL<sub>4</sub>, XeF<sub>4</sub>, XeCI<sub>4</sub>.

- 1. E.A.V Ebsworth; W.H Renkin; Cradock, Structure Methods in InorganicChemistry.
- 2. R.S Drago, Physical Methods for Chemists (Ist and IInd Edition).
- 3. C.N Banwell, Fundamentals of MolecularSpectroscopy.
- 4. S. Walker and H. Straugh an Spectroscopy, Vol.I.
- 5. J.E. Wertz & J.R. Bolton, Electron Spin Resonance(p.49-65).
- 6. N.N. Greenwood & T.C Tibb, MossbauerSpectroscopy.
- 7. K. Nakamoto, Infrared Spectra of Inorganic and co-ordinationCompounds.

## Master of Science (Chemistry)(Semester-II) Session: 2021-22 COURSE CODE: MCHL-2336 COURSE TITLE: MATHEMATICS FOR CHEMISTS (For Medical Students)

#### **Course outcomes:**

Students will be able to acquire knowledge about

CO1: trigonometry

- CO2: determinants and matrices
- CO3: integration and differentiation

## Master of Science (Chemistry) (Semester-II) Session: 2021-22 COURSE CODE: MCHL-2336 COURSE TITLE: MATHEMATICS FOR CHEMISTS (For Medical Students)

Time:2 Hrs.

Max. Marks: 25

(Theory: 20, CA: 5)

# Note: The students are allowed to use Non-Programmable Calculator. Instructions for the Paper Setters:

Eight questions of equal marks( four each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from anySection.

#### UNIT-I

#### **Trigonometry and Determinants:**

Definition of sin, cos, tan, cot, sec, cosec functions with the help of unit circle, values of sin x, cos x for x =  $\frac{0}{\pi}/6_{\pi}/3$ ,  $\frac{12}{\pi}$ . Trigonometric identities (without proofs) and their applications. Definition and expansion properties of determinants, product of two determinants of 3rd order.

#### UNIT-II

#### Matrices:

Introduction to various forms of Matrices, row, column, diagonal UNIT, Submatrix, square, equal matrices, null, symmetric and skew symmetric matrices, transpose of a matrix, adjoint and inverse of matrices. Addition, multiplication, characteristic equation of a matrix, statement of Cayley Hamilton theorem. Rank of matrix, condition of consistency of a system of linear equations. Eigen vectors and Eigen valuesofmatrices.

#### UNIT-III Differential Calculus

Differentiation of standard functions, theorems relating to the derivative of the sum, difference, product and quotient of functions (without proofs), derivative of trigonometric functions, inverse trigonometric functions, logarithmic functions and exponential functions, differentiation of implicit functions, logarithmic differentiation.

## UNIT-IV Integral Calculus

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 as limit of a sum and geometrical interpretation.

- 1. Santi Narayan & P.K. Mittal DifferentialCalculus.
- 2. Santi Narayan & P.K. Mittal IntegralCalculus.
- 3. B.S. Grewal Higher EngineeringMathematics.
- 4. Joseph B. Dence Mathematical Techniques inChemistry.
- 5. Margenau and Murphy, the MathematicsofPhysics and Chemistry.
- 6. B.L. Moncha and H.R. Choudhary A Text Book of EngineeringMathematics.

## Master of Science(Chemistry)(Semester-II) Session: 2021-22 COURSE CODE: MCHL-2057 COURSE TITLE: BIOLOGY FORCHEMISTS (For Non-Medical Students)

## **Course outcomes:**

Students will be able to understand

CO1: organization of life

CO2: genetics

CO3: diversity of life

Master of Science (Chemistry) (Semester-II)

## Session: 2021-22 COURSE CODE: MCHL-2057 COURSE TITLE: BIOLOGY FORCHEMISTS (For Non-Medical Students)

## Time:2 Hrs.

## Max. Marks: 25

(Theory: 20, CA: 5)

## Note 1: The students are allowed to use Non-Programmable Calculator.

## **Instructions for the Paper Setter**

Eight questions of equal marks (four each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from anySection.

## UNIT-I

## The Organisation of Life

Biologically important molecules: Carbohydrates, lipids, proteins and nucleicacids. 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.

## **UNIT-II**

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

## UNIT-III

**Genetics:** The basic principle of heredity: Mendals law, monohybrid cross, dihybridcross.DNA – Double helix structure and replication.Genes expression: Transcription and translation, geneticcode.

## UNIT-IV

**The Diversity of Life:** The classification of Living things – Criteria of classification, Whittaker's systems of classification, their characteristics with are example of each. Viruses, structure of Viruses.

## **Book Recommended:**

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

## Master of Science (Chemistry)(Semester-II) SESSION: 2021-22 COURSE CODE:MCHP-2088 (PRACTICAL)

## **Course outcomes:**

The students will be able to

CO1: understand and perform multi step organic synthesis.

CO2: expertise the various techniques of analysis of organic substances

## Master of Science (Chemistry) (Semester-II) Session: 2021-22 COURSE CODE: MCHP-2088 COURSE TITLE: ORGANIC CHEMISTRY (PRACTICAL)

## Time:6 Hrs

#### Max. Marks: 75 (P: 60, CA: 15)

**Instruction for practical examiner:** Question paper is to be set on the spot jointly by the Internal and External Examiners. Two copies of the same should be submitted for the record to COE Office, Kanya Maha Vidyalaya, Jalandhar

## A. Multistep Organic Synthesis

- 1. Synthesis of 2-chloro-4-bromoaniline from aniline (Bromination and chlorination) Book 1, page292.
- 2. Synthesis of methyl orange fromaniline. (Aromatic electrophilic substitution and diazocoupling).Book 2, page 250.
- 3. Synthesis of benzpinacol and its pinacolrearrangement.
- 4. Synthesis of o-chlorobenzoic acid from phthalimide. Synthesis of acridone from ochlorobenzoic acid. (Hofmann bromamide and Sandmeyer'sreaction).
- 5. Synthesis of 2,4-dinitrophenyl hydrazine from chloro benzene. (Electrophilic and nucleophilic substitution reactions on aromaticring).
- 6. Synthesis of triphenylcarbinol from bromobenzene. (Grignard reaction) Book 2, page220.

## **B:** Quantitative Analysis of Organic Compounds:

- Estimation of phenol/aniline using bromate-bromidesolution. (The application to find the purity of the sample and to determine the amount in given solution).
- 2. Determine the number of hydroxyl and amino groups in the given sample by the acetylation method.
- 3. Determine the mol. wt. of the given ketone by using 2,4-DNPmethod.
- 4. Estimation of reducing sugar by Fehling solutionmethod.
- 5. To determine the saponification value of the given fat or oilsample.
- 6. To determine the iodine number of the given fat or oilsample.

- 1. An Introduction to Modern Experimental Organic Chemistry, R. M. Roberts, J. C. Gilbert, L.B.Rodewald and A. S. Wingrove Holt, Ranehart and Winston Inc. NewYork.
- Introduction to Organic Laboratory Techniques A Contemporary Approach. D. L.Pavia, G. M. Lampmana and G. S. Kriz, W. B. Saunders Company, 1976.
- 3. Laboratory Experiments in Organic Chemistry, R. Adams, J. R. Johnson and C. F. Wilcox. The Macmillan Limited,London.

4. Text Book of Practical Organic Chemistry, A. I.Vogel.

## Master of Science (Chemistry)(Semester-II) Session: 2021-22 COURSE CODE: MCHP-2089 COURSE TITLE:Physical Chemistry(Practical)

#### **Course outcomes:**

Students will be able to

CO1: prepare for each experiment by studying lab handouts and links therein

CO2: know about the safety requirements and lab skills required to perform physico-chemical

experiments

CO3: design and perform experiments to determine the rate, order, and activation

energy of chemical reactions by varying concentrations and/or temperature

CO4: carry out preparation of buffer solutions at a required pH, given a choice of solutions of

acid/conjugate base pairs

CO5: know the principle and mechanism of Conductometric titrations and polarimetric experiments CO6: determine specific and molar refraction using Abbe's refractometer

## Master of Science (Chemistry)(Semester-II) Session: 2021-22 COURSE CODE:MCHP-2089 COURSE TITLE: Physical Chemistry(Practical)

## Time:6 Hrs

## Max. Marks:75

## (P: 60, CA: 15)

**Instruction for practical examiner:** Question paper is to be set on the spot jointly by the Internal and External Examiners. Two copies of the same should be submitted for the record to COE Office, Kanya Maha Vidyalaya, Jalandhar.

- 1) To determine the strength of given acid by pHmetrically.
- 2) To determine dissociation constant of given acid pHmetrically
- 3) Titration of weak acid conductometrically
- 4) Titration of strong acidconductometrically
- 5) To determine dissociation constant of given acidconductometrically
- 6) Determine the dissociation constant of acetic acid in DMSO, DMF, dioxane by titratingit with KOH.
- 7) Determine the activity coefficient of an electrolyte at different molalitiesbye.m.f. measurements.
- 8) Compare the cleansing powers of samples of two detergents from surfacetension measurements.
- 9) Determine the specific refraction, molar refraction and atomic parachor with the helpofAbbe'srefractometer.
- **10)** To study the distribution of benzoic acid between benzene andwater.
- **11)** Determine the equilibrium constant of reaction K1 +12 à K13 by distribution lawand hence find the value of go of the abovereaction.
- **12)** Compare the relative strength of CH<sub>3</sub>COOH and CICH<sub>2</sub>COOH from conductance measurements.
- **13)** Determine the solubility (g/litre) of sparingly soluble lead sulphate fromconductance measurements.
- **14)** Titrate a given mixture of HCl and CH<sub>3</sub>COOH against NaOH solution conductometrically.
- **15)** Compare the relative strengthof:
- i) HCl and ii) H<sub>2</sub>SO<sub>4</sub> by following the kinetics of inversion of cane sugarPolarimetrically.

#### **Books Recommended:**

1.Yadav, J. B (2005): *Advanced Practical Physical Chemistry*, 22<sup>nd</sup> edition, Goel publishing House, Krishna Prakashan Media Ltd.

2. Venkatesan, V, Veeraswamy, R and Kulandaivelu, A.R (1997): *Basic Principles of Practical Chemistry*", 2nd edition, Sultan Chand and Sons Publication, New Delhi.

#### Master of Science (Chemistry) (Semester-III)

#### Session: 2021-22

## **COURSE CODE: MCHL-3081**

## **COURSE TITLE: Inorganic Chemistry-II**

## (Theory)

#### **Course outcomes:**

Students will be able to

CO1: know about the various metal ions present in our body, their function in body and role in medicine

CO2: learn about the different enzymes participating in the chemical reactions inside the

body and their functions

CO3: study about the different oxygen carriers present in the body with their structure and stereochemistry

CO4: study in detail about nitrogen fixation reactions and microorganisms involved in nitrogen fixation reactions

# Master of Science (Chemistry)(Semester-III) Session: 2021-22 COURSE CODE: MCHL-3081 COURSE TITLE: Inorganic Chemistry-II

(Theory)

Time: 3 Hrs

Max. Marks: 50

(Theory: 40, CA: 10)

## Note: The students are allowed to use Non-Programmable Calculator.

## **Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITS I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

## UNIT-I

**Metal Ions in Biological Systems-** Essential and trace elements, periodic survey of essential and trace elements, biological importance and relative abundance, Na+/ K+ ion pump.

**Transport and Storage of Dioxygen**- Oxygen carriers-Hb and Mb: Structure and mechanism of their function, co-operativity, inhibition and poisoning by ligands and metal ions, hemocyanins and hemerythrin, model complexes of iron, cobalt and copper.

## UNIT-II

**Bioenergetics and ATP Cycle-** Process concept to phosphate hydrolysis, Nucleotide transfer- DNA polymerase, phosphate transfer pyruvate kinase, phosphoglucomutase, created kinase, ATPase **Photosynthesis and respiration** – chlorophyll : structure, function and its synthetic model.

**Bioredox Agents and Mechanism-** Enzymes and their functioning, Vitamin  $B_{12}$  coenzyme, its function and application in organic syntheses, intake of alcohol and its remedy.

## UNIT-III

Biochemistry of Iron- Availability of iron, competition for iron, iron toxicity and nutrition.

**Electron Transfer in Biology**- Cytochromes-structure and function, CN- and CO poisoning, Ferredoxin and rubredoxim. **Nitrogenase**- Biological  $N_2$  fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases modelsystems.

Metal Storage, Transport- Ferritin, transferring and siderophores.

**UNIT-IV** 

Metalloenzymes- Zinc enzymes-carboxypeptidase and carbonic anhydrase, Copper enzymes- superoxide dismutase.

**Calcium in Biology-** Calcium in living cell, transport and regulation, molecular aspects of intramolecular processes,

Metals in Medicine- Metal deficiency and disease, toxic effects of antibiotics and related compounds, chelate therapy

- 1. Principles of Bioinorganic Chemistry, S. J. Lippard and Berg, University ScienceBooks.
- 2. Inorganic Biochemistry, Vol I and II. Ed. G. L. Eichhorn, Elsevier.
- 3. J.E. Huheey : Inorganic Chemistry III & IV Ed. Pearson Education Asia –(2002).
- 4. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 5thEdition.
- 5. Progress in Inorganic Chemistry, Vols 18 and 38 Ed. J. J. Lippard, Wiley
- 6. Bioinorganic Chemistry by D.Banergia

## (Semester-III)

#### Session: 2021-22

#### COURSE CODE: MCHL-3082

## **COURSE TITLE:Organic Synthesis**

#### (Theory)

#### **Course outcomes:**

Students will be able to

CO1: understand general mechanistic consideration of organic rearrangements

CO2: understand synthesis and reactions of macroring compounds and fused polynuclear hydrocarbons

CO3: study the synthesis and reactions of three, four, six, seven and large membered Heterocycles

CO4: know about the use of various reagents in organic synthesis and functional group transformations

CO5: understand the basic concepts of supramolecular chemistry

## (Semester-III)

#### Session: 2021-22

## **COURSE CODE: MCHL-3082**

## **COURSE TITLE:Organic Synthesis**

## (Theory)

Time: 3 Hrs

Max. Marks: 50

(Theory: 40, CA: 10)

## Note: The students are allowed to use Non-Programmable Calculator.

## **Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

## UNIT-I

**Rearrangements**: General mechanistic considerations – nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements: Pinacol-pinacolone, Wagner-Merwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofmann, Curtius, Schmidt, Baeyer-Villiger, Shapiroreaction.

## Polynuclear Compounds & Macro-Ring Compounds

Introduction, comparative study of aromatic character of Linear and non-Linear-ortho-fused polynuclear hydrocarbons, ortho-and peri-fused polynuclear hydrocarbons.General method of preparation and reactions of indene, fluorene anthracene and phenanthrene. Modern methods of synthesis of macro ring compounds-civiton, muscone and catenanes.

#### UNIT-II

## **Heterocyclic Synthesis**

Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reaction.

#### **Small Ring Heterocycles**

Synthesis of aziridines, oxiranes, thiiranes and their ring opening and rearrangement reactions.

#### **Five-Membered Heterocycles with one Heteroatom**

Synthesis of Furan, Pyrrole, Thiophene and their electrophilic, nucleophilic, metallation reactions.

## Six-Membered Heterocycles with one Heteroatom

Pyridine synthesis (from dicarbonyl compounds, *HantzschSynthesis, through cycloaddition reactions*), reactions of pyridine (electrophilic, nucleophilic, metallation), synthesis of pyrylium salts, pyrones, benzopyrylium

salts, benzopyrones (coumarins, chromones) and their electrophilic, nucleophilic and addition reactions, reactivity of pyrylium and benzopyrylium salts, pyrones and benzopyrones.

## Seven-and Large-Membered Heterocycles

Synthesis and reactions of azepines, oxepines, thiepines, thiazepines.

## UNIT-III

## **Reagents in Organic Synthesis**

Use of the following reagents in organic synthesis and functional group transformations; Complex metal hydrides, Gilman's reagent, lithium dimethylcuprate, lithium disopropylamide (LDA) dicyclohexylcarbodimide. 1,3-Dithiane (reactivity umpolung), trimethylsilyl iodide, tri-n-butyltinhybride, Woodward and prevost hydroxylation, osmium tetroxide, DDQ, selenium dioxide, phase transfer catalysts, crown ethers and Merrifield resin, Peterson's synthesis, Wilkinson's catalyst, Bakeryeast.

## **UNIT-IV**

## Supramolecular Chemistry

Definition and development of supramolecularchemistry, Classification of supramolecular Host- Guest compounds, Historical concepts such as receptors, coordination, lock and key analogy, Chelate and Macrocyclic effects, Preorganization and Complementarity, Thermodynamics and Kinetic selectivity, Overview of intermolecular forces such as Hydrogen bonding, Hydrophobic effects, Cation- $\pi$  interactions, Ion-ion, Ion-dipole, Dipole-dipole interactions,  $\pi$ - $\pi$  stacking, van der Waals forces, Synthesis and structure of supramolecular hosts for Recognition of cations: Crown ethers, Cryptands, Spherands, Siderophores; for Recognition of anions: Guanidinium- based receptors; for Recognition of neutral molecules: Cyclotriveratrylene (CTV).

- 1. Supramolecular Chemistry, Jonathan W. Steed, Jerry L. Atwood, John Wiley & Sons
- 2. Principles of Modern Hetrocyclic Chemistry by L.A. Paquette
- 3. Hetrocyclic Chemistry by J.A. Joule and K. Mills
- 4. Heterocyclic Chemistry by Gilrchirst

## (Semester-III)

## Session: 2021-22

## **COURSE CODE: MCHL-3083**

## **COURSE TITLE: Surface and Polymer Chemistry**

## (Theory)

#### **Course outcomes:**

Students will be able to

CO1: study concept of adsorption and micelle formation

CO2: learn about the different kinetics and thermodynamics of polymerization

CO3: learn about the type and classification of polymers

CO4: know about the structure, properties and utilization of polymers.

CO5: study in detail about the glass transition temperature

## (Semester-III)

## Session: 2021-22

## COURSE CODE: MCHL-3083 COURSE TITLE: Surface and Polymer Chemistry

#### (Theory)

Time: 3 Hrs

Max. Marks: 50

(Theory: 40, CA: 10)

## Note: The students are allowed to use Non-Programmable Calculator.

## **Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

#### UNIT-I

## Adsorption

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

#### UNIT-II Micelles

Surface active agents, classif

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 – phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

## UNIT-III Macromolecules

**Polymer** – definition, types of polymers, electrically conducting, fire resistant, liquids crystal polymers, kinetics of polymerization, thermodynamics of polymerization.

Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculations of average dimensions of various chain structures. Importance of polymers, Basic concepts: monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers. Polymerization: condensation, addition, radical chain-ionic and co-ordination and copolymerization. Polymerization conditions and polymer reactions.Polymerization in homogenous and heterogeneous systems. Number, weight and viscosity average weights.

## UNIT IV

## **Structure and Properties:**

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 polymerutilization.

- 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 Publishers, Moscow

#### (Semester-III)

#### Session: 2021-22

#### **COURSE CODE: MCHL-3084**

#### **COURSE TITLE: Electrochemistry and Chemical Dynamics**

#### (Theory)

#### **Course outcomes:**

Students will be able to

CO1: Understand the electrochemistry of solutions, method of determination of electrified interfaces, semiconductor electrolyte solution interface

CO2: know theory, monitoring and prevention of corrosion

CO4: understand collision theory of reaction rates, Arrhenius theory and activated complex theory, Lindemann-Hinshelwood theory

CO5: understand various Photochemical reactions, Homogeneous catalysis and kinetics of enzyme reactions, general features and methods of studying fast reactions

CO6: interpret spectra and applications of Voltammetry and Polarography.

Master of Science (Chemistry)

(Semester-III)

#### Session: 2021-22

#### **COURSE CODE: MCHL-3084**

#### **COURSE TITLE: Electrochemistry and ChemicalDynamics**

#### (Theory)

Time: 3 Hrs

Max. Marks: 50

(Theory: 40, CA: 10)

#### Note: The students are allowed to use Non-Programmable Calculator.

#### **Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

#### UNIT-I

**Electrochemistry**Electrochemistry of solutions, Debye-Huckel-Onsager treatment and its extension, ion-solvent interactions, Debye-Huckel-Bjerrum mode, Thermodynamics of electrified interface equation, Derivation of electro-capillarity, Lipmann equation(surface ecess), method of determination, structure of electrified interfaces, Guoy-Chpmann, Stern models, over potential, 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, homogeneous theory, forms of corrosion, corrosion monitoring and prevention

#### UNIT-II

#### **Chemical Dynamics (A)**

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 unimolecular reactions, Lindemann-Hinshelwood theory. Dynamic Chain (hydrogen bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane),

#### UNIT-III

#### **Chemical Dynamics (B)**

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 Voltammetry and Polarography

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

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

#### **Master of Science (Chemistry)**

#### (Semester-III)

#### Session: 2021-22

#### **COURSE CODE: MCHL-3085**

#### **COURSE TITLE: Photochemistry and Pericyclic reactions**

#### (Theory)

#### **Course outcomes:**

Students will be able to

CO1: classify the pericyclic reactions and explain them under thermal and photochemical conditions.

CO2: interpret the product of Pericyclic reactions (Cyclo addition, Electocyclic and sigmatropic Reactions)

CO3: know the basic concepts of photochemical reactions and determine their reaction mechanisms

CO4: apply the knowledge of photochemical reactions of Alkenes, carbonyl compounds, aromatic compounds.

CO5:study named photochemical reactions, photochemistry of smog, polymers and vision

**Master of Science (Chemistry)** 

(Semester-III)

Session: 2021-22

#### **COURSE CODE: MCHL-3085**

#### **COURSE TITLE: Photochemistry and Pericyclic reactions**

(Theory)

Time: 3 Hrs

Max. Marks: 50

(Theory: 40, CA: 10)

Note: The students are allowed to use Non-Programmable Calculator.

#### **Instructions for the Paper Setters:**

Eight questions of equal marks (eight each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

#### UNIT-1

#### **Pericyclic Reactions** (A)

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 he explanation of pericyclic reactions under thermal and photo-chemical conditions. Electrocyclic reactions – controtatory and disrotatory motions, 4n, 4n+2, allylsystems secondary effects. Cycloadditions – antrafacial and suprafacial additions, notation of cylcoadditions (4n) and (4n+2) systems with a greater emphasis on (2+2) and (4+2)

#### UNIT-II

#### **Pericyclic Reactions (B)**

cycloaddition-stereochemical effects and effects of substituents on the rates of cycloadditions, 1,3-dipolar cyclo-additions and cheleotropicreactions.Sigmatropic Rearrangements-suprafacial and antrafacial shifts [1,2]- sigmatropic shifts involving carbon moieties retention and invertion 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. Elecrocyclic rearrangement of cyclobutenes and 1,3cyclohexadienes.

## **UNIT-III**

#### Photochemistry

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

## **Determination of Reaction Mechanism**

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-phasephotolysis.

## **UNIT-IV**

#### **Photochemistry of Alkenes**

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

## **Photochemistry of Carbonyl Compounds**

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.

## **Photochemistry of Aromatic Compounds**

Isomerisations, additions and substitutions.

## **Miscellaneous Photochemical Reactions**

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

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

## Master of Science (Chemistry)

## (Semester-III)

## Session: 2021-22

## COURSE CODE: MCHP-3086

## **COURSE TITLE: Inorganic Chemistry Practical (Preparations)**

#### **Course outcomes:**

Students will be able to

CO1: plan and Conduct experiments for synthesizing, analysing, identifying and characterizing inorganic compounds

CO2: do measurements of magnetic moments of synthesized complexes.

CO3: estimate metal content in the synthesized complex

#### **Master of Science (Chemistry)**

#### (Semester-III)

#### Session: 2021-22

#### **COURSE CODE: MCHP-3086**

#### **COURSE TITLE: Inorganic Chemistry Practical (Preparations)**

Time: 6 hrs.

Max. Marks: 75 (P: 60, CA: 15)

**Instruction for practical examiner:** Question paper is to be set on the spot jointly by the Internal and External Examiners. Two copies of the same should be submitted for the record to COE Office, Kanya Maha Vidyalaya, Jalandhar.

- Preparation of Co(acac)<sub>3</sub>, its characterization using NMR, IR, UV-Vis and analysis of Cobalt. (ref. J. Chem. Edu., 1980, 57, 7,525)
- 2. Preparation of Co(acac-NO<sub>2</sub>)<sub>3</sub>, its characterization using NMR, IR, UV-Vis and analysis of Cobalt. (ref. J. Chem. Edu., 1980, 57, 7,525)
- Preparation of [Fe(H<sub>2</sub>O)<sub>6</sub>][Fe(N-salicyldeneglycinato)<sub>2</sub>]<sub>2</sub>.3H<sub>2</sub>O, its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Iron.(ref. InorganicaChimicaActa, 1977, 23,35).
- 4. Preparation of [Ni(NH<sub>3</sub>)<sub>6</sub>]Cl<sub>2</sub> its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Nickel and NH<sub>3</sub>. (ref. Marr and Rockett,1972).
- 5. Preparation of [Ni(ethylenediamine)<sub>3</sub>]Cl<sub>2</sub> its characterization using IR, UV-Vis, magnetic susceptibility and analysis of Nickel. (ref. Marr and Rockett, 1972, page270).
- Preparation of [Fe(NO)(S<sub>2</sub>CN(Et)<sub>2</sub>)<sub>2</sub>] 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).
- 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 VO(acac)<sub>2</sub> 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 ofCopper(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,

page386).

- 11. Preparation of HgCo(NCS)<sub>4</sub> , its IR and measure its magnetic moment. (ref. Marr andRockett, 1972, page365).
- 12. Preparation of sodium tetrathionate, interpretation of its IR and analysis using potassium iodate. (ref. Marr and Rockett, 1972, page214).
- 13. Preparation of Potassium dithionate, interpretation of its IR and analysis using potassium iodate. (ref. Marr and Rockett, 1972, page214).
- 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-tetraazacyclo tetradeca-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, page386).

- 1. B.N. Figgis, Introduction to Ligand Field, WileyEastern.
- 2. A.B.P. Lever, Inorganic Electronic Spectroscopy, Elsevier.
- 3. A.Earnshaw, Introduction to Magnetochemistry, AcademicPress.
- 4. J.E. Huheey, Inorganic Chemistry Principles of Structure and Reactivity, Harper Interscience.
- 5. R.S. Drago, Physical Medhod in Chemistry, W.B.SaundersCompany.
- 6. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, WileyInterscience.
- 7. F.A. Cotton, Chemical Application of Group Theory, WileyEaster

## Master of Science (Chemistry)

## (Semester-III)

## Session: 2021-22

## **COURSE CODE: MCHP-3087**

## **COURSE TITLE: Physical Chemistry Practical**

#### **Course outcomes**

Students will be able to

CO1: apply the principle and mechanism of Conductometric and potentiometric titrations

CO2: determine the partial molar volumeof compounds using Dilatometer

CO3: determine specific and molar refractivity using Abbes refractometer

CO4: study complex formation and the kinetics of hydrolysis Spectrophotometrically

CO5: determine the molecular weight of polymers byviscometry

## Master of Science (Chemistry)

## (Semester-III)

## Session: 2021-22

## **COURSE CODE: MCHP-3087**

## **COURSE TITLE: Physical Chemistry Practical**

Time: 6 Hrs.

Max. Marks: 75 (P: 60, CA: 15)

**Instruction for practical examiner:** Question paper is to be set on the spot jointly by the Internal and External Examiners. Two copies of the same should be submitted for the record to COE Office, Kanya Maha Vidyalaya, Jalandhar.

- 1. To determine the partial molar volume of (a) Glycine (b) Urea using dilatometer
- To determine the partial molar volumeof

   (a) methanol
   (b) n-propanol usingdilatometer
- 3. To determine the surface tension (double capillary) of mixture of solid and water by deferential method and hence find out parachor of themixture.
- 4. To determine the specific and molar refractivity of n-propanol, butanol, hexane and carbon tetrachloride and calculate refraction equivalents of C, H andCl.
- 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 molefraction.
- 6. To determine the equivalent conductance of weak electrolyte (acetic acid) at infinite dilution using Kohlrauschlaw.
- 7. Determine equivalent conductance of strong electrolyte at several concentrations and hence verify Onsagerequation.
- 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 theelectrolyte.
- 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 violetspectrophotometrically.
- 13. To determine the pH of various mixtures of sodium acetate and acetic acid in aqueous solution and hence determine the dissociation constant of theacid.
- 14. Titrate potentiometrically Zn(II) by  $K_4Fe(CN)_6$  and verify the composition of the complex  $K_2Zn_3[Fe(CN)_6]_2$
- 15. Determination of nitrite in water spectrophotometrically.
- 16. Determination of molecular weight of polymers by Viscometry.
- 17. Determine the molar refraction of a solid substance by dissolving it in a solvent and its refractive index.

1. Yadav, J. B (2005): *Advanced Practical Physical Chemistry*, 22<sup>nd</sup> edition, Goel publishing House, Krishna Prakashan Media Ltd.

2. Venkatesan, V., Veeraswamy, R. and Kulandaivelu, A.R (1997): *Basic Principles of Practical Chemistry*", 2nd edition, Sultan Chand and Sons Publication, New Delhi.

## Session: 2021-22 COURSE CODE: MCHL-4081 COURSE TITLE: Advanced Inorganic Chemistry(Theory)

#### **Course outcome:**

Students will be able to

CO1: understand Franck-Condon principle

CO2:understand Photo substitution reactions, photoredox reactions, photolysis of water

CO3:oxidative addition and reductive elimination, migration (Insertion) reaction and cyclometallation reactions,

CO4:characterise the compound by synthetic methods and know the chemical behaviour and synthetic applications of hydride compounds

CO4:understandhydroformylation, Carbonylation Reaction, decarbonylation reactions, hydrocyanation Polymerization, Oligomerisation and metathesis reactions and Oxidation reaction

## Session: 2021-22 COURSE CODE: MCHL-4081 COURSE TITLE: Advanced Inorganic Chemistry (Theory)

#### Time: 3 Hrs

Max. Marks: 75

(Theory: 60, CA: 15)

#### Note: The students are allowed to use Non-Programmable Calculator.

#### **Instructions for the Paper Setters:**

Eight questions of equal marks (twelve each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

#### UNIT-I

#### **Photo Inorganic Chemistry:**

Basics of photochemistry- Absorption, excitation, photochemical laws, quantum yield, electronically excited states, life times- measurements of the times Flash photolysis, energy diddipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, photochemical stages-primary and secondary processes, Kashia's rule, Thexi state, Photo substitution reactions, Adamson's rules, Photo substitution reactions of Cr(III)-Polypyridyls, Rh(III) Ammine Complexes, Ru-Polypyridyl complexes, Ligand photo reactions, photoredox reactions, comparison of Fe(II) and Ru(II) complexes, Photo reactions and Solar energy conversions, Photo synthesis in plants and Bacterio chlorophyll photosynthesis, photolysis of water using Inorganic precursors.

#### UNIT-II

#### **Oxidative-Addition and Migration (Insertion Reactions):**

Introduction: Acid base behaviour of metal atoms in complexes, Protonation and Lewis Base behaviour, acceptor properties of Lewis acidity of complexes, oxidative addition and reductive elimination, addition of specific molecules, Hydrogen addition, HX additions, Organic halides addition of some other molecules productive elimination, migration (Insertion) reaction 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>, RCM, Insertion of alkenes and C-C unsaturated compounds, Cleavage of C-H bonds; alkane activation, Cyclometallation reactions. Reactions of free hydrocarbons.

### UNIT-III

### Transition Metal Compounds with Bonds to Hydrogen

Characteristics of hydride complexes, synthetic methods, chemical behaviour of hydride compounds, mononuclear polyhydrides, homolepticpolyhydride anions; carbonyl hydrides and onion. Molecular hydrogen compounds; metal hydrogen interaction with C-H bonds; MH interactions; complexes of boron hydride and aluminohydrides, synthetic applications of metal hydrides.

### **UNIT-IV**

### **Transition Metal Complexes in Catalysis:**

Hydroformylation of unsaturated compounds, Reductive carbonylation of alcohols and other compounds; Carbonylation Reaction: Methanol and methyl acetate, Adipic ester. Synthesis and other carbonylation reactions, decarbonylation reactions. Catalytic addition of molecules to C-C multiple bonds homogeneous hydrogenation, hydrocyanation of unsaturated compounds, hydrosilation of unsaturated compounds, hydrocyanation of alkenes, Polymerization, Oligomerisation and metathesis reactions of alkenes and alkynes, Ziegler-Natta polymerisation of ethylene and propylene oligomerisation and related reactions, Cluster compounds in catalysis, supported homogeneous and phase transfer catalysis, Oxidation reaction: Oxidative carbonylations, Palladium catalysed oxidation of ethylene, Acrylonitrile synthesis, oxygen transfer from peroxo- and oxo- species, oxygen transfer from NO<sub>2</sub>groups.

- 1. Concepts of Inorganic Photochemistry, A. W. Adamson and P. D. Fleischauer, Wiley.
- 2. W.W. Porterfield, Inorganic Chemistry: A Unified Approach.
- 3. F.A. Cotton and G. Willkinson, Advanced Inorganic Chemistry, 5thed, John Wiley & Sons, NewYork.
- C.ElschenbroichandA.Salzer,Organometalics:AConciseIntroduction,2ndEd.,VCH 1992.

## Master of Science (Chemistry)(Semester-IV) Session: 2021-22 COURSE CODE: MCHL-4082 COURSE TITLE: Chemistry of Natural Products (Theory)

#### **Course outcome:**

Students will be able to

CO1: study the biosynthetic pathways of natural products

CO2:Understand the isoprene rule and its role in terpenoids

CO3:Classify and understand the synthesis and structure of steroids and alkaloids

CO4:understand the chemistry of Haemin, chlorophyll, prostaglandins and antibiotics

CO5: classify and elucidate the structure of carbohydrates like starch and cellulose

CO6:determine thestructure conformation and properties of proteins

CO7:determine the structure of nucleic acids DNA and RNA

## Master of Science (Chemistry)(Semester-IV) Session: 2021-22 COURSE CODE: MCHL-4082 COURSE TITLE: Chemistry of Natural Products (Theory)

Time: 3 Hrs CA: 15) Max. Marks: 75 (Theory: 60,

### Note: The students are allowed to use Non-Programmable Calculator

#### **Instructions for the Paper Setters:**

Eight questions of equal marks (twelve each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section. **UNIT-1** 

### **Studies on Biosynthetic Pathways of Natural Products**

The acetate hypothesis, poly-ketoacids, their aldol type cyclisations and meta orientations of hydroxyl groups in naturally occurring phenols. b) Isoprene rule, mechanism of formation of mevalonic acid from acctyl 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 abieticacid.

#### UNIT-II

#### Terpenoids

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

#### Steroids

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

#### Alkaloids

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

## UNIT-III

#### Haemin and Chlorophyll

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

## Antibiotics

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

### Prostaglandins

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

## UNIT-IV

#### Carbohydrates

Nomenceature and classification, types of naturally occuring sugars, deoxy sugars, sugars, methyl others and acid derivatives of sugars. General methods of structure and ring size determination, structure of maltose, lactose, sucrose, starch and cellulos.

## **Peptides and Proteins**

Sequence determination insulin and oxytocin, Proteins: structure conformation and properties. Enzymes, Kinetics, inhibition mechanism.

# Nucleic Acids

Nucleosides, nucleotides, DNA, RNA structure and conformation, Replication, transcription.

- 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. Fundamentals of BioChemistry by D. Voet, J.G. Voet and C.W.Pratt, John Wiley & Sons Inc., New York, 1999.
- 5. Principles of Biochemistry by A.L. Lehninger, CBS Publishers, New Delhi

## Master of Science (Chemistry)(Semester-IV) Session: 2021-22 COURSE CODE: MCHL-4083 COURSE TITLE: Chemistry of Materials

### **Course outcome:**

Students will be able to

CO1:understand types of solids, point defects, electrical properties and conduction in metals

CO2: understand reactions in organic solids, photochemical reactions and decomposition and dehydration reactions.

CO3:explain the properties and applications of different types of polymers.

CO4: define the factors affecting glass formation, types, properties and applications of different types of glasses

CO5:learn glass ceramic compositions, properties and applications

CO6:predict the methods of preparation of smart materials, types of superconductors and their applications

## Master of Science (Chemistry)(Semester-IV) Session: 2021-22 COURSE CODE: MCHL-4083 COURSE TITLE: Chemistry of Materials (Theory)

Time: 3 Hrs

Max. Marks: 75

(Theory: 60, CA: 15)

## Note: The students are allowed to use Non-Programmable Calculator.

#### **Instructions for the Paper Setters:**

Eight questions of equal marks (twelve each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from UNITs I-IV of the syllabus respectively. Questions may be subdivided into parts (not exceeding four). Candidates are required to attempt five questions, selecting at least one question from each section. The fifth question may be attempted from any Section.

## UNIT-I

#### Solid State Chemistry

Types of solids, band and bond theories, crystal lattice energy, point defects in metals and ionic compounds, energy and entropy of defects, their concentration, diffusion and electrical conduction via defects, nonstoichiometric types, colourcenters and electrical properties of alkali halides, electron theories for metal conduction in metals, in insulators, impurity semiconductors, reactions in organic solids, photochemical reactions, solid-solid reactions, decomposition and dehydrationreaction. **UNIT-II** 

#### Macromolecules

Types of polymers, regular and irregular polymers, synthesis of polymers by chain and step reactions, physical properties of solid polymers(crystallinity, plasticity and elasticity), vulcanization of rubbers, molecular mass determination by osmometric, viscometry, light scattering and ultracentrifuge methods, number and mass average molecular masses, polymer solutions, factors affecting the solubility of polymers , conducting polymers, doping of polymers, mechanism of conduction, polarons and bipolarons,

## UNIT-III

#### **Glasses and Ceramics**

Factors affecting glass formation, oxide glasses, electronegativity and bond type, viscosity, structural effects(zachariasen's rule(1932), criteria of SUN and Rawson, thermodynamics of glass formation, behavior of liquids on cooling, kinetics of crystallization and glass formation, structure of glasses: vitreous silica, silicate glasses, vitreous B2O3 and borate glasses, viscosity, electrical conductivity of glasses and the mixed alkali effect, commercial silicate and borate glasses, metallic glasses , glass ceramics, refractories, important glass-ceramics compositions, properties of glass ceramics, applications.

**UNIT-IV** 

**Smart Materials** 

Methods of preparation- conventional ceramic methods, hot pressing and hot static pressing techniques, precursor method, gel method, co-precipitation method, glass crystallization methods, vacuum techniques- chemical vapor deposition method. organic superconductors, magnetism in organic materials, magnetic nano materials, energy storage materials, nano materials for targeted drug delivery, fullerenes as superconductors. High temperature ceramic superconductors, electrical and magnetic properties of superconductors, critical temperature Tc, thermodynamics of superconductors, London equation, BCS theory, applications.

- 1. Principles of polymer chemistry—P J Flory Cornell UniversityPress
- 2. Physical chemistry of polymers—A J Tager, MirPublishers
- 3. Physical chemistry of MacromoleculesTanford
- 4. Handbook of conducting polymers—T ASkotthem
- 5. Solid state physics—A J Dekker- MacMillanPublishers
- 6. Solid state chemistry and its applications—A R West ,WileyPublishers
- 7. Solid state chemistry of drugs S R ByrnAcademicPress
- 8. Chemistry of solid state—W.E.GarnerButterworth
- 9. Principles of physical chemistry—Puri-Sharma-Pathania, VishalPublishers
- 10. Thermotropic Liquid crystals Ed. G W Gray JohnWiley
- 11. Chemistry of polymers, MargarisonandEast
- 12. Polymer Chemistry, Malcolm, P, Stevens, Oxford UniversityPress
- 13. Principles of Solid States, H. V. Keer, WileyEastern.

## Session: 2021-22 COURSE CODE: MCHP-4084 COURSE TITLE: Advanced Practical- Organic Synthesis

#### **Course outcome:**

Students will be able to

CO1:plan and implement advance organic synthesis and reactions

CO2:characterize organic molecules by physical and spectroscopic means, including M.P, B.P, and IR

CO3: predict the outcome and mechanism of some simple organic reactions, using a basic understanding of the relative reactivity of functional groups

## Session: 2021-22 COURSE CODE: MCHP-4084 COURSE TITLE: Advanced Practical- Organic Synthesis

Time: 6 Hrs.

Max. Marks: 50 (P: 40, CA: 10)

**Instruction for practical examiner:** Question paper is to be set on the spot jointly by the Internal and External Examiners. Two copies of the same should be submitted for the record to COE Office, Kanya Maha Vidyalaya, Jalandhar.

- 1. Synthesis and Reactivity ofbenzalacetophenone
  - a. Bromination (Electrophilic additions) &subsequentdebromination (Elimination)
  - b. Epoxidation (Cycloaddition, nucleophilic) and ring opening with hydroxideion.
  - c. Michael addition of aniline.
  - d. Conversion of benzalacetophenone to its oxime (nucleophilic addition atC=O)
  - e. Conversion of oxime to amide (Beckmann rearrangement) and oxazole (Understand the reactivities at conjugated C=O and C=C)bond.
- 2. 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 withKMnO<sub>4</sub> (Mechanism of *syn*- and *anti*-cyclohexane-1,2-diol)
- 3. Preparation and characterization of the Aldol-dehydration products from various combinations of aromatic aldehydes andketone.

Effect of substituents on aromatic aldehydes on the product distribution.

- a. Aldehyde:benzaldehyde, 4-methylbenzaldehyde.4-methoxybenzaldehyde.
- b. Ketone: acetone, cyclopentanons, cyclohexanone (Book4)6.

- 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 OrganicChemistry.
- 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.

## Master of Science (Chemistry)(Semester-IV) Session: 2021-22 COURSE CODE: MCHP-4085

## **COURSE TITLE: Advanced Practical- Inorganic Synthesis**

### **Course outcome:**

Students will be able to

CO1: apply key concepts of inorganic chemistry and coordination compounds including those related to synthesis, reaction chemistry, and structure and bonding

CO2:design the basic and advanced laboratory procedures used in inorganic synthesis including spectroscopic and analytical techniques for identification and characterization of small molecules

CO3: learn separation of metal cations by chromatographic techniques

## Master of Science (Chemistry) (Semester-IV) Session: 2021-22 COURSE CODE: MCHP-4085

#### **COURSE TITLE: Advanced Practical- Inorganic Synthesis**

Time: 6 Hrs.

Max. Marks: 50 (P: 40, CA: 10)

**Instruction for practical examiner:** Question paper is to be set on the spot jointly by the Internal and External Examiners. Two copies of the same should be submitted for the record to COE Office, Kanya Maha Vidyalaya, Jalandhar.

- 1. Synthesis of the Linkage Isomers nitrito- and nitropentaamminecobalt(III)chloride
  - a) Preparation of chloropentaamminecobalt(III) chloride, [Co(NH<sub>3</sub>)<sub>5</sub>Cl]Cl<sub>2</sub>.
  - b) Preparation of nitropentaamminecobalt(III) chloride, [Co(NH<sub>3</sub>)<sub>5</sub>(NO<sub>2</sub>)]Cl<sub>2</sub>.
  - c) Preparation of nitritopentaamminecobalt(III) chloride, [Co(NH<sub>3</sub>)<sub>5</sub>(ONO)]Cl<sub>2</sub>.
  - d) Estimate the chloride in all the complexes using gravimetricanalysis.
  - e) Record and interpret the electronic absorption spectra and IR spectra of allcobalt(III) complexes and assign the observed change to distinguish the twoisomers.
- 2. Synthesis of a coordination compound containing iron and analysis of thiscompound using redoxmethods
  - a) Preparation of iron(II)oxalate
  - b) Preparation of  $K_3$  [Fe(C<sub>2</sub>O<sub>4</sub>)<sub>3</sub>].3H<sub>2</sub>O
  - c) Characterization of Iron(II) and iron(III) complex with IRspectroscopy
  - d) Determination of iron and oxalate in  $K_3[Fe(C_2O_4)_3]$ .3H<sub>2</sub>O using volumetricanalysis
- 3. Synthesis and characterization of the Ni(II) complex of a Schiff-base ligand derived from Salicylaldehyde and ethylenediamine.
  - a) Synthesis the Schiff-baseligand.
  - b) Interpret the 1H NMR and IR spectra of theligand.
  - c) Synthesis the Ni(II) complex of the ligand and compare its IR spectrum with thatoftheligand.
- 4. Separation of the metal cationsby
  - a) Column chromatography with gradient elution Co(II) and Ni(II). Analyze qualitatively the coloured fractions collected for separatedcations.
  - b) Paper chromatography [Fe(II), Co(II), Ni(II) and Cu(II). Determine the Rf values for the separate standard cations and use these to identify the cations present in the unknownmixture.

- 1. G. Marr, B. W. Rockett, Practical Inorganic Chemistry(1972).
- 2. I. Grenthe, E. Nordin, Inorganic Chemistry, 18 (1979)1869-74.
- 3. J.C. Bailar, M. Eldon, Inorg. Synth. 1 (1939)35-38.

## Master of Science (Chemistry)(Semester-IV) Session: 2021-22 COURSE CODE: MCHP-4086 COURSE TITLE: Advanced Practical- Physical Chemistry

### **Course outcome:**

Students will be able to

CO1:experience the scientific methods employed in basic and applied physical chemistry

CO2: design and perform experiments to determine the rate, order, and activation energy of chemical reactions by varying concentrations and/or temperature

CO3: measure equilibrium concentrations and equilibrium constants for acid-base, solubility, and complexation reactions given initial concentrations of reactant

CO4: develop skills in procedures and instrumental methods like polarography, turbidimetry and spectrophotometry,

## Master of Science (Chemistry) (Semester-IV) Session: 2021-22 COURSE CODE: MCHP-4086 COURSE TITLE: Advanced Practical- Physical Chemistry

Time: 6 Hrs.

Max. Marks: 50 (P: 40, CA: 10)

**Instruction for practical examiner:** Question paper is to be set on the spot jointly by the Internal and External Examiners. Two copies of the same should be submitted for the record to COE Office, Kanya Maha Vidyalaya, Jalandhar.

## CHEMICAL EQUILIBRIUM

- 1. Study the effect of solvent on the conductance of AgNO<sub>3</sub>/Acetic acid and determine the degree of dissociation and equilibrium constant in different solvents and their mixtures (DMSO, DMF, dioxane, acetone, and water) and test the validity of DEBYE- HUCKEL-ONSAGER'Sequation.
- 2. To determine acid and base dissociation constant of amino acid pHmetrically.
- 3. To calculate thermodynamic parameters G,  $\Delta Sand$  H for the reaction,  $Zn + Hg_2SO_4$   $2Hg + Zn SO_4$  by emfmeasurement.

## CHEMICAL KINETICS

- 4. Study the salt effects and the solvent effect on the rate law of alkaline hydrolysis of crystal violet.
- 5. Determine the degree of hydrolysis and hydrolysis constant of CH<sub>3</sub>COONa/NaCl/aniline hydrochloride.
- 6. Determine the order of reaction by analyzing the kinetic dependence of individual reactant (e.g. saponification of ester).
- 7. Determine the energy of activation for the reaction studied above.

## ACTIVITY AND ACTIVITY COEFFICIENTS

- 8. Determination of mean activity coefficient of given electrolyte bycryoscopy.
- 9. Determine activity coefficients by EMFmethod.

## PHASE EQUILIBRIUM

- 10. Draw the phase diagram for any one of the following three componentpartially immiscible liquidsystems.
   i) DMSO/water/benzena
   ii) water/benzena/actionaid
  - i) DMSO/water/benzene ii) water/benzene/aceticacid

## **POLAROGRAPHIC TECHNIQUES**

- 11. Estimation of ions in mixture of Pb2+ and Cd2+ by successive reduction. Evaluate diffusion coefficient of Cd2+
- 12. Polarographic determination of Cu and Zn in the given sample of brass.
- 13. Determine stability constants of Cd2+ with EDTA.

#### **SPECTROPHOTOMETRIC METHODS**

14. To study the effect of extended conjugation on the wave length ofmaximum absorption of organic compounds.

#### **ADSORPTION**

1. To determine the adsorption isotherms of heavy metals like Cd, Zn, Cr, Pb. Ni by using nonconventional adsorbents.

#### TURBIDITYMETRY

- 2. To determine concentration of sulphate ions with the help of turbiditymeter.
- 3. Determine the CMC by turbidimetricmethod.
- 4. Preparation of soap and determination of its CMC.

#### LEAST SQUARE FITTING

5. To draw calibration curve for the concentration determination of potassium ions by flame photometry and to study the least square fitting of thedata.

#### **Books Recommended:**

1.Yadav, J. B (2005): *Advanced Practical Physical Chemistry*, 22<sup>nd</sup> edition, Goel publishing House, Krishna Prakashan Media Ltd.

2. Venkatesan, V,Veeraswamy, R and Kulandaivelu, A.R (1997): *Basic Principles of Practical Chemistry*", 2nd edition, Sultan Chand and Sons Publication, New Delhi.

3. Findlay's (1985): *Practical Physical Chemistry*, Revised and edited by B.P. Levitt 9 th edition, Longman, London.

4. Chatwal, G.R. and Anand, S.K (2000): *Instrumental Methods of Chemical Analysis*, Himalaya Publishing House, Delhi.