

FACULTY OF SCIENCES

SYLLABUS

of

Master of Science (Chemistry)

(Semester: I - IV)

(Under Credit Based Continuous Evaluation Grading System)

Session: 2022-24



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)

Credit Based Continuous Evaluation Grading System (CBCEGS)

(Session: 2022-2024)

Semester I

Master of Science (Chemistry) Semester I										
Course Code	Course Title	Course Type	Hours Per Week L-T-P	Credits L-T-P	Total Credits	Marks				Examination time (in Hours)
						Total	Th	P	CA	
MCHL-1081	Ligand Field Theory	C	4-0-0	4-0-0	4	50	40	-	10	3
MCHL-1082	Organic Reaction Mechanism-I	C	4-0-0	4-0-0	4	50	40	-	10	3
MCHL-1083	Physical Chemistry – Thermodynamics	C	4-0-0	4-0-0	4	50	40	-	10	3
MCHL-1084	Spectroscopy A: Techniques for Structure Elucidation of Organic Compounds	C	4-0-0	4-0-0	4	75	60	-	15	3
MCHM-1135	Computer for Chemists	IDC	2-0-2	2-0-1	3	75	40	20	15	3+3
MCHP-1086	Inorganic Chemistry Practical (Quantitative Analysis)	C	0-0-6	0-0-3	3	75	-	60	15	3*2

MCHP-1087	Organic Chemistry Practical	C	0-0-6	0-0-3	3	75	-	60	15	3*2
Student can opt any one of the following Interdisciplinary compulsory courses		IDE			4					
Total				25		450				
IDEC-1101*	Effective Communication Skills		4-0-0			100	80	-	20	3
IDEM-1362*	Basics of Music (Vocal)		2-1-1			100	40	40	20	
IDEH-1313*	Human Rights and Constitutional Duties		4-0-0			100	80	-	20	
			2-0-4			100	50	30	20	3+3
IDEI-1124*	Basics of Computer Applications		4-0-0			100	80	-	20	3
IDEW-1275	Indian Heritage: Contribution to the world									
(*Credits of these ID courses will not be added to SGPA)										

C- Compulsory Course

IDE- Inter Disciplinary Elective Course

IDC-Inter Disciplinary Compulsory Course

Programme Specific Outcomes

On successful completion of this Programme, students will have ability to:

PSO1: do global level research, pursue Ph.D. programme and targeted approach of CSIR-NET examination and competitive exams conducted by service commission

PSO2: attain enormous job opportunities at all levels of chemical, pharmaceutical, food products and life oriented material industries.

PSO3: get recruitment in R and D and synthetic division of polymer industries and Allied division.

PSO4: apply modern methods of analysis to chemical systems in a laboratory setting.

PSO5: work effectively and safely in a laboratory environment, use technologies/instrumentation to gather and analyse data and work in teams as well as independently.

PSO6: think critically, develop scientific temper and analyse various chemical.

Master of Science (Chemistry)
(Semester-I)
Session 2022-24
COURSE CODE: MCHL-1081
Course Title: Ligand Field Theory

Course outcomes:

Students will be able to

CO1: learn mathematical rules for the formation of symmetry point groups

CO2: construct the Character table for various point groups and to determine the symmetry of hybrid orbitals

CO3: analyze Tanabe – Sugano /Orgel diagrams and determine the magnetic properties of complexes.

CO4: analyze and understand the electronic spectra of octahedral and tetrahedral metal complexes.

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Master of Science (Chemistry)
(Semester-I)
Session: 2022-24
COURSE CODE: MCHL-1081
COURSE TITLE: Ligand field Theory

Time: 3Hrs
Credit (L-T-P): 4-0-0

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 σ and π 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 character Tables.

UNIT-II

Molecular Orbital Theory for Metal Complexes:

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 σ and π bonding in transition metal complexes.

Interelectronic Repulsions:

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 (λ) energy separation between different j states, The effect of octahedral and tetrahedral fields on S, P, D and F terms (with help of the character table), splitting patterns of and G, H and I terms

UNIT-III

Free Ions in Medium and Strong Crystal Fields:

Strong field configurations, transition from weak to strong crystal fields, evaluation of strong crystal field terms of d^2 configuration in octahedral and tetrahedral crystal fields (using group

theory), construction of the correlation energy level diagrams of d^2 configuration in octahedral field, study of energy level diagrams for higher configurations, selection rules of electronic transitions in transition metal complexes, their proof using group theory, relaxation of the selection rule in centrosymmetric and non-centrosymmetric molecules, Orgel diagrams, Tanabe Sugano diagrams

Magnetic Properties:

Van Vleck's formula for susceptibility, first order Zeeman effect, second order Zeeman effect, KT states, quenching of orbital 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^n metal ions.

UNIT-IV

Electronic Spectra of Transition Metal Complexes:

Variation of the Racah parameter, nephelauxetic effect -central field covalency, symmetry restricted covalency, differential radial expansion, spectrochemical series, band intensities, factors influencing band widths, discussion of electronic spectra of octahedral and tetrahedral d^1 – d^9 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_3MoCl_6 and $[Rh(NH_3)_6]^{3+}$, spectra of cis and trans $[Co(en)_2X_2]^+$, $[Mn(H_2O)_6]^{2+}$, $CuSO_4 \cdot 5H_2O$ and its anhydrous complex, comparison of d–d band with f–f bands. Introduction to Charge Transfer Spectra.

Books Recommended:

1. F.A. Cotton, Chemical Application of Group Theory, Wiley Eastern.
2. G. L. Miessler, D. A. Tarr, Inorganic Chemistry, 3rd edition, Pearson Education.
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. Saunders Company.
8. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Wiley Inter-science.

Master of Science (Chemistry)
(Semester-I)
Session: 2022-24
COURSE CODE: MCHL-1082
COURSE TITLE: Organic Reaction Mechanism- I

Course outcomes:

Students will be able to

CO1: understand the concept and various types of aromaticity and acquire the skills for correct stereochemical assignment and interpretation in simple organic molecules.

CO2: basics of reaction mechanism and understand the various types of aliphatic nucleophilic substitution reaction and their mechanism

CO3: understand the various types of aliphatic nucleophilic substitution reaction and discuss their mechanism and predict the product of the reactions

CO4: understand the various types of aromatic electrophilic and nucleophilic substitution reaction and their mechanism alongwith identification and application of various rearrangement reactions

Master of Science (Chemistry)
(Semester-I)
Session: 2022-24
COURSE CODE: MCHL-1082
COURSE TITLE: Organic Reaction Mechanism- I

Time: 3Hrs

Max. Marks: 50

Credit (L-T-P): 4-0-0

(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

Nature of Bonding in Organic Reactions:

Aromaticity in Benzenoid and non-benzenoid compounds. Huckel's Rule, Alternant and non-alternant hydrocarbons. Energy levels of $\pi(\text{pi})$ 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 SN^2 , SN^1 and SNi mechanisms, mixed SN^1 and SN^2 mechanism SET mechanism. The neighboring group mechanism (anchimeric assistance). Neighboring group participation by π and sigma bonds.

UNIT-III

Aliphatic Nucleophilic Substitution – B:

Classical, non-classical and 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 Substitution:

Bimolecular mechanism – S_E2 and S_Ei. The S_E1 mechanism, Hydrogen exchange, electrophilic substitution accompanied by double bond shifts, diazo-transfer reaction, formation of sulphur ylides, 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, Vilsmeier reaction, Gattermann-Koch reaction, Pechmann reaction, Houben – Hoesch reaction, Fries rearrangement.

Aromatic Nucleophilic Substitution:

S_NAr, S_N¹, benzyne and S_{RN}¹ mechanisms. Reactivity effect of substrate structure, leaving group and nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

Books Recommended:

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

Master of Science (Chemistry)
(Semester-I)
Session: 2022-24
COURSE CODE: MCHL-1083
COURSE TITLE: Physical Chemistry – Thermodynamics

Course outcomes:

Students will be able to

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

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

CO3: 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, explain T^3 dependence of heat capacity of solids at low temperatures (universal feature) using Debye and Einstein theory of heat capacity of solids.

CO4: understand non-equilibrium states, apply Onsager's reciprocity relations and irreversible thermodynamics for biological systems.

Master of Science (Chemistry)
(Semester-I)
Session: 2022-24
COURSE CODE: MCHL-1083
COURSE TITLE: Physical Chemistry –Thermodynamics

Time: 3Hrs

Max. Marks: 50

Credit (L-T-P): 4-0-0

(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 stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electro kinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

Books Recommended:

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: 2022-24
COURSE CODE: MCHL-1084
COURSE TITLE: SPECTROSCOPY – A: Techniques in Structure Elucidation of Organic Compounds

Course outcomes:

Students will be able to

CO1: know about the Nuclear magnetic resonance spectroscopy. Proton chemical shift, spin-spin coupling, coupling constants and its applications to determine organic structures

CO2: to understand different cleavage patterns of organic compounds in Mass spectrometry and apply the knowledge for interpretation of the spectrum of an unknown compound and the principle and applications of ultraviolet and apply Woodward Fisher Rule to calculate λ_{\max}

CO3: understand the concepts of Vibrational spectroscopy, Vibrational coupling overtones and Fermi resonance and its application in Organic Chemistry

CO4: apply NMR, IR, MS, UV-Vis spectroscopic techniques in solving structure of organic molecules and in determination of their stereochemistry.

Master of Science (Chemistry)
(Semester-I)
Session: 2022-24

COURSE CODE: MCHL-1084

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

Time: 3Hrs
Credit (L-T-P): 4-0-0

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

Nuclear Magnetic Resonance

The Nuclear spin, Larmor frequency, the NMR isotopes, population of nuclear spin level, spin and spin lattice relaxation. Measurement techniques (CW and 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 ^1H . - 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

Mass Spectroscopy

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, Retro-Diels-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 Visible Spectroscopy

The energy of electronic excitation, measurement techniques, Beer-Lambert Law, Molar extinction coefficient. The Franck-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

Infrared Spectroscopy

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

Applications in Organic Chemistry

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

UNIT-IV

1. Solution of Structural Problems by Combined Use of the following Spectroscopic Techniques:

- (a) Electronic spectra
- (b) Vibrational spectroscopy
- (c) NMR (^1H) spectroscopy
- (d) Mass Spectroscopy

Books Recommended:

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

Master of Science (Chemistry)
(Semester-I)
Session: 2022-24
COURSE CODE: MCHM-1135
COURSE TITLE: Computer for Chemists

Course outcomes:

The students will be able to:

CO1: Comprehend various programming constructs like variables, data-types, operators, etc of C programming language.

CO2: Apply various control statements of C Programming Language for designing solutions to different real world problems.

CO3: Comprehend signature, declaration, definition and calling of functions in C for modularization of problem.

CO4: Implement single and multidimensional arrays for representing complex data collections.

Master of Science (Chemistry)
(Semester-I)
Session: 2022-24
COURSE CODE: MCHM-1135
COURSE TITLE: Computer for Chemists

Time: (3+3)Hrs
Credit (L-T-P): 3-0-1

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:

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 C language

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 in Chemistry

(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 linear regression.
4. Calculation of curve linear regression.

UNIT-II

5. Calculation of Bohr orbit from de Broglie Lambda for electron.
6. Calculation of wave number and frequency from value of wavelength.
7. Calculation of van der Waals radii.
8. Radioactive decay.
9. Rate constant of a 1st order reaction, 2nd order reaction.
10. Calculation of lattice energy using Born Lande equation.

UNIT-III

11. Addition, multiplication and solution of inverse of 3 X 3 matrix.
12. Calculation of average molecular weight of a polymer containing n_1 molecules of molecular weight m_1 , n_2 molecules of molecular weight m_2 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 diatomic molecule.
15. Calculate the RMS and most probable velocity of a gas.

UNIT-IV

16. Calculate the ionic mobility from ionic conductance values.
17. Determine the thermodynamic parameters for isothermal expansion of monoatomic ideal gas.
18. Calculation of value of g- factor from value of J and S.
19. Calculate the bond length and bond angles using crystal structure data.

Books Recommended:

1. K.V. Raman, Computers in Chemistry, Tata McGraw Hill, 1993.
2. Henry Mullish, Herbert L. Cooper, The Spirit of C: An Introduction to Modern Programming, Jaico Publications, 1987.
3. Anshuman Sharma, Learn Programming in C, Lakhanpal Publishers, 7th Edition.
4. E Balagurusamy, Programming in ANSI C, Tata McGraw-Hill, 2002.
5. Yashvant Kanetkar, Let Us C, BPB Publications, 2016.
6. Byron Gottfried, Schaum's Outline Programming with C, McGraw Hill, 1996.

Note: The latest editions of the books should be followed.

Master of Science (Chemistry)
(Semester-I)
Session: 2022-24
COURSE CODE: MCHP-1086
COURSE TITLE: INORGANIC CHEMISTRY (PRACTICAL)
(Quantitative Analysis)

Course outcomes:

Students will be able to

CO1: Experimental observation of Inorganic Quantitative Analysis

CO2: determine the strength of ions by Oxidation reduction titrations

CO3: estimate the amount of ions by precipitation titrations

CO4: estimate the amount of ions by complexometric and gravimetric methods

Master of Science (Chemistry)
(Semester-I)
Session: 2022-24
COURSE CODE: MCHP-1086
COURSE TITLE: INORGANIC CHEMISTRY (PRACTICAL)
(Quantitative Analysis)

Time: 6 Hrs

Max. Marks: 75

Credit (L-T-P): 0-0-3

(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-Reduction Titrations

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^- and $\text{C}_2\text{O}_4^{2-}$ ions.
3. Standardization of $\text{K}_2\text{Cr}_2\text{O}_7$ with Fe^{2+} and determination of Fe^{3+} (Ferricalum)
4. Standardization of hypo solution with potassium iodate / $\text{K}_2\text{Cr}_2\text{O}_7$ and determination of available Cl_2 in bleaching powder, Sb^{3+} and Cu^{2+} .
5. Determination of hydrazine with KIO_3 titration.

II. Precipitation Titrations

1. AgNO_3 standardization by Mohr's method by using adsorption indicator.
2. Volhard's method for Cl^- determination.
3. Determination of ammonium / potassium thiocyanate.

III. Complexometric Titrations

1. Determination of Mg^{2+} and Mn^{2+} in a mixture using fluoride ion as a demasking agent.
2. Determination of Ni^{2+} (back titration).
3. Determination of Ca^{2+} (by substitution method).

IV. Gravimetric Analysis

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

Books Recommended:

Vogel's book on Inorganic Quantitative Analysis

Master of Science (Chemistry)
(Semester I)
Session: 2022-24
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 natural products

Master of Science (Chemistry)
(Semester I)
Session: 2022-24
COURSE CODE: MCHP-1087
COURSE TITLE: ORGANIC CHEMISTRY
(PRACTICAL)

Time: 6Hrs

Max. Marks: 75

Credit (L-T-P): 0-0-3

(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 TLC plates.
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 purify 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 reactions/proteins).
3. *Synthesis of 2-phenylindole-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, methyl 3-nitrobenzoate.
5. *Cannizzaro's reaction of 4-chlorobenzaldehyde*. Book 1, p.760
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-chlorobenzaldehyde, 4-chlorobenzoic acid 4-chlorobenzyl alcohol.
6. *Synthesis of 1,3,5-Tribromobenzene from aniline*. **Aim:** To demonstrate: Bromination, Diazotization and Reduction.

Books Recommended:

Vogel's Text book of practical organic chemistry, 5th edition.

KANYA MAHA VIDYALAYA JALANDHAR (AUTONOMOUS)

SCHEME AND CURRICULUM OF EXAMINATION OF TWO YEAR DEGREE PROGRAMME

Master of Science (Chemistry)

Credit Based Continuous Evaluation Grading System (CBCEGS)

(Session: 2022-2023)

Semester II

Master of Science (Chemistry) Semester II										
Course Code	Course Title	Course Type	Hours Per Week L-T-P	Credits L-T-P	Total Credits	Marks				Examination time (in Hours)
						Total	Th	P	CA	
MCHL-2081	Organometallics Chemistry	C	4-0-0	4-0-0	4	50	40	-	10	3
MCHL-2082	Organic Reaction Mechanism -II	C	4-0-0	4-0-0	4	50	40	-	10	3
MCHL-2083	Physical Chemistry – Quantum Chemistry	C	4-0-0	4-0-0	4	50	40	-	10	3
MCHL-2084	Reaction Mechanisms and Metal clusters	C	4-0-0	4-0-0	4	50	40	-	10	3
MCHL-2085	Spectroscopy B: Techniques for Structure Elucidation of Inorganic Compounds	C	4-0-0	4-0-0	4	75	60	-	15	3
MCHL-2336 MCHL-2057	Mathematics for Chemists Biology for Chemists	IDE	2-0-0	2-0-0	2	25	20	-	5	3

MCHP-2088	Organic Chemistry Practical	C	0-0-6	0-0-3	3	75	-	60	15	3*2
MCHP-2089	Physical Chemistry Practical	C	0-0-6	0-0-3	3	75	-	60	15	3*2
Total					28	450				

C- Compulsory Course

IDE- Inter Disciplinary Elective Course

IDC-Inter Disciplinary Compulsory Course

Master of Science (Chemistry)
(Semester-II)
Session: 2022-24
COURSE CODE: MCHL-2081
COURSE TITLE: ORGANOMETALLICS CHEMISTRY

Course outcomes:

Students will be able to

CO1: demonstrate basic principles and illustrate stability of organometallic compounds.

CO2: identify the structure and bonding aspects of simple organometallic compounds

CO3: identify different types of organometallic reactions and apply the above concepts to explain different catalytic reactions

CO4: understand the role of pi acid ligands in organometallic chemistry

Master of Science (Chemistry) (Semester-II)
Session: 2022-24
COURSE CODE: MCHL-2081
COURSE TITLE: ORGANOMETALLICSCHEMISTRY

Time: 3Hrs

Max. Marks: 50

Credit (L-T-P): 4-0-0

(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

Organometallics

Energy polarity and reactivity of M-C bond, Stability of Main group organometallics: Methods of preparation in perspective-organolithium compounds: structure and bonding and 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. η^2 - ligands: olefinic and acetylenic complexes, chelating olefinic ligands – synthesis and structure. η^2 – ligands: Allylic and η^4 – complexes of cyclopentadiene.

UNIT-II

Synthesis and structure. η^4 –ligands: Butadiene, cyclobutadiene, heterocyclic pentadiene (S, Se, Te). Classification, Nomenclature of cyclopentadienyl complex. MO treatment of ferrocene. η^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, O₂, N₂, NO, PH₃ 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.

Books Recommended:

1. C. Elschenbroich and A. Salzer, Organometallics: A Concise Introduction, 2ndEd., VCH 1992.
2. J.E. Huheey, Inorganic Chemistry Principles of Structure and Reactivity, Harper Interscience.
3. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Ed. V and VI. Wiley Interscience.
4. G. L. Miessler, D. A. Tarr, Inorganic Chemistry, 3rd edition, Pearson Education

Master of Science (Chemistry) (Semester-II)
Session: 2022-24
COURSE CODE: MCHL-2082
COURSE TITLE: Organic Reaction Mechanism – II

Course outcomes:

Students will be able to

CO1: understand the types, mechanism and factors affecting free radical reactions, apply the knowledge to predict the product of free radical reactions and to obtain an outline about elimination reactions and some specific examples of elimination reactions

CO2 : understand the mechanistic and stereochemical aspects of addition to Carbon – Carbon multiple bonds alongwith the reaction and mechanism of some named reactions of this type

CO3: understand the mechanism of metal hydride reduction of saturated/ unsaturated organic compounds learn its basic mechanism and to predict the mechanism of condensation reactions involving enolates and reactions involving carbon- carbon bond formation

CO4: acquire knowledge about the reagents used for oxidation and reduction of various organic compounds

Master of Science (Chemistry)
(Semester-II)
Session: 2022-24
COURSE CODE: MCHL-2082
COURSE TITLE: Organic Reaction Mechanism – II

Time: 3Hrs

Max. Marks: 50

Credit(L-T-P): 4-0-0

(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 any Section.

UNIT-I

1.Free Radical Reactions

Types of free radical reactions, free radical substitution mechanism. Mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. 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 Multiple Bonds

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.

UNIT-III

5. Addition to Carbon – Hetero Multiple Bonds –B

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

6. Formation of Carbon-Carbon Bond

Principle, disconnections and synthons, electrophilic and nucleophilic carbon species. Base-catalyzed condensations; Aldol condensation, Claisen reaction, Perkin reaction, Stobbe condensation, Darzen condensation. Use of malonic, acetoacetic and cyanoacetic esters, Micheal addition, 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.

Books Recommended:

1. Principles of Organic Synthesis – Norman and Coxon
2. Advanced Organic Chemistry – Jerry March.
3. Advanced Organic Chemistry, F.A. Carey, R.J.Sunberg.
4. Highlights of Organic Chemistry, W, J.L. Nobel; An Advanced Text Book.
- 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 William Carruthers

Master of Science (Chemistry)
(Semester-II)
Session: 2022-24
COURSE CODE: MCHL-2083
COURSE TITLE: Physical Chemistry-Quantum Chemistry

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, apply this knowledge to atomic structure

CO2: use mathematical 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

CO3: relate concepts that were originally introduced purely as modern atomic physics to molecular systems through harmonic oscillator, spin and rigid rotator

CO4: solve all 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.

Master of Science (Chemistry)
(Semester-II)
Session: 2022-24
COURSE CODE: MCHL-2083
COURSE TITLE: Physical Chemistry – Quantum Chemistry

Time: 3 Hrs

Credit(L-T-P): 4-0-0

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

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 quantum mechanics.

UNIT-III

3. Applications of Quantum Postulates

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, cyclobutadiene cyclopropenyl system.

6. The Approximate Methods

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

Books Suggested:

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

Master of Science (Chemistry)

(Semester-II)

Session: 2022-24

COURSE CODE: MCHL-2084

COURSE TITLE: REACTION MECHANISMS AND METAL CLUSTERS

Course outcomes:

Students will be able to

CO1: learn the mechanism of substitution reaction and explain the parameters that affects the crystal structure of a compound

CO2: learn the application of electron transfer reactions in chemical kinetics

CO2: describe the stability of metal complexes by the use of formation constants

And calculate thermodynamic parameters from them

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

Master of Science (Chemistry)

(Semester-II)

Session: 2022-24

COURSE CODE: MCHL-2084

COURSE TITLE: REACTION MECHANISMS AND METAL CLUSTERS

Time: 3Hrs.

Max.Marks:50

Credit(L-T-P): 4-0-0

(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 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 organometallic compounds, trigonal bipyramid, system with six or more coordination number. Isomerization and racemization 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 spectrophotometry.

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 and sulphides, Higher boranes and carboranes, methods of classifying boranes, Molecular orbit view of chlorohydroborane ions and carboranes, metallocarboranes, isopoly and heteropoly acids and salts; metal-metal bonds and bi-, tri-, tetra-, penta-, and hexanuclear clusters, electron counting schemes for HNC's. Approaches to systematic cluster synthesis; mention of seven, eight and nine atom clusters. Isolobal analogy and examples of application of analogy.

Books Recommended:

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, 3rd edition, Pearson Education.
3. F.A. Cotton and Wilkinson: Inorganic Chemistry V and VI Ed. Wiley Eastern – (1999).
4. J.E. Huheey: Inorganic Chemistry III and IV Ed. Pearson Education Asia – (2002).

Master of Science (Chemistry)
(Semester-II)
Session: 2022-24
COURSE CODE: MCHL-2085
COURSE TITLE: SPECTROSCOPY – B: Techniques for Structure Elucidation of Inorganic Compounds

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: 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: 2022-24
COURSE CODE: MCHL-2085
COURSE TITLE: SPECTROSCOPY – B: Techniques for Structure
Elucidation of Inorganic Compounds

Time: 3Hrs

Max. Marks: 75

Credit (L-T-P): 4-0-0

(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

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 bands. Group vibrations and limitations of group vibration concepts.

UNIT – II

Vibration and Rotation Spectroscopy: Infrared, Raman and Microwave

- Polarisation 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, vibronic coupling.

- Sample handling. Factors affecting absorption frequencies. Interpretation and finger printing regions. Use of symmetry considerations to determine the number of active I.R., and Raman lines (character tables to be provided in the Examination)

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UNIT-III

(A) Applications

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

(i) Metalcarbonyls. (ii) NSF_3 (iii) Geometrical isomerism – differentiation between Cis and

trans. $[\text{Co}(\text{bipy})_2\text{Cl}_2]\text{Cl}$. (iv) Structures of CO_2 , N_2O , H_2O , chlorocomplexes of mercury, cadmium and zinc and some octahedral complexes ML_6 (eg. SiF_6^{2-} , PF_5^- , SF_6). (v) Changes in the spectra of donor molecules upon coordination with special emphasis on N, N – dimethyl – acetamide and DMSO with Fe^{3+} , Cr^{3+} , Zn^{2+} , Pd^{2+} and Pt^{2+} ions. I.R spectroscopy and modes of coordination of SO_4^{2-} , N_2 , O_2 , NO , CO_3^{2-} , NO_3^- .

(B) Photo Electron Spectroscopy

Introduction, excitation and ejection of electrons, electronic energy levels in atoms and molecules, Core level photoelectron spectroscopy, symmetry and 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 , $\text{C}_{14}\text{H}_{10}$, biphenyl) Anisotropic splitting, Electron – electron interaction, Transition metal complexes g-value and factors affecting g-value, zero field splitting, Kramer's degeneracy, Rate of electron exchange, Application to p – benzoquinone 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 eQ, double resonance technique, Application ($\text{PFCl}_4.\text{PCl}_5$), $(\text{NH}_4)_2\text{TeCl}_6$, group 14 tetra halides, R_3MX_2 ($\text{M}=\text{As}, \text{Sb}, \text{Bi}$), Cis and Trans $[\text{Co}(\text{en})_2\text{Cl}_2]\text{Cl}$, Polyhalide ion, BrCN , HIO_3 (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 $\{^{57}\text{Fe}, ^{119}\text{Sn}, ^{151}\text{Eu}\}$ compounds, to biological systems to surface study, I_2Cl_6 , IBr_2Cl_4 , XeF_4 , XeCl_4 .

Books Recommended:

1. E.A.V Ebsworth; W.H Renkin; Craddock, Structure Methods in Inorganic Chemistry.
2. R.S Drago, Physical Methods for Chemists (1st and 2nd Edition).
3. C.N Banwell, Fundamentals of Molecular Spectroscopy.
4. S. Walker and H. Strauss Spectroscopy, Vol.I.
5. J.E. Wertz and J.R. Bolton, Electron Spin Resonance (p.49-65).
6. N.N. Greenwood and T.C Tibb, Mossbauer Spectroscopy.
7. K. Nakamoto, Infrared Spectra of Inorganic and co-ordination Compounds.

Master of Science (Chemistry) Semester-II

Session 2022-24

Course Title: Mathematics for Chemists

Course Code-MCHL-2336

Course outcomes:

Students will be able to

CO 1: Understand the trigonometric functions with the help of unit circle and application of trigonometric identities and able to solve determinants with the help of its various properties.

CO 2: Demonstrate the concept of matrices and type of matrices and how to calculate transpose, adjoint and inverse of matrices. Manage to solve problems related to addition, subtraction and multiplication. To understand the concept and solve system of linear equations.

CO 3: Solve Complex problems related to derivative of sum, difference, product and quotient of functions and also to find derivative of trigonometric functions, inverse trigonometric functions, logarithmic functions and exponential functions.

CO 4: Recognize integration as an inverse of differentiation and to calculate area under curve and understand integrals as limit of sum and its geometrical interpretation.

Master of Science (Chemistry)
(Semester-II)
Session: 2022-24
COURSE CODE: MCHL-2336
COURSE TITLE: MATHEMATICS FOR CHEMISTS
(For Medical Students)

Time: 3 Hrs

Max. Marks: 25

Credit (L-T-P): 2-0-0

(Theory: 20, CA: 5)

Instructions for the Paper Setters:

Eight questions of equal 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 any Section.

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 $x = 0, \pi/6, \pi/3, \pi/2$. 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 values of matrices.

Unit-III

Differential Calculus

Differentiation of standard functions, theorems relating to 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, area under a curve, indefinite integrals of standard forms, method of substitution, method of partial fractions, integration by parts, definite integrals, definite integrals as limit of a sum and geometrical interpretation.

Reference Books:

1. Mathematics Textbook for class XI, NCERT
2. Mathematics Textbook for class XII, NCERT
3. J. B. Dence, Mathematical Techniques in Chemistry, John Wiley & Sons, First edition, 1975.

Master of Science (Chemistry)
(Semester-II)
Session: 2022-24
COURSE CODE: MCHL-2057
COURSE TITLE: BIOLOGY FORCHEMISTS
(For Non-Medical Students)

Course outcomes:

Students will be able to

CO1: Gain knowledge about the biomolecules and cell structure.

CO2: Understand different types of tissues.

CO3: Understand Mendelian laws, structure of DNA and gene expression.

CO4: Understand Whittaker's system of classification and structure of virus.

Master of Science (Chemistry)
(Semester-II)
Session: 2022-24
COURSE CODE: MCHL-2057
COURSE TITLE: BIOLOGY FOR CHEMISTS
(For Non-Medical Students)

Time: 3 Hrs

Max. Marks: 25

Credit (L-T-P): 2-0-0

(Theory: 20, CA: 5)

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

Instructions for the Paper Setter

Eight questions of equal marks (4 marks each) are to be set, two in each of the four Sections (A-D). Questions of Sections A-D should be set from unit 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

The Organization of Life

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

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

UNIT-II

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

UNIT-III

Genetics

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

DNA – Double helix structure and replication.

Genes expression: Transcription and translation, genetic code.

UNIT-IV

The Diversity of Life

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

Viruses, structure of Viruses.

Book Recommended:

1. Cord Biology - South Western Educational Publications, Texas, 200

Master of Science (Chemistry)
(Semester-II)
Session: 2022-24
COURSE CODE: MCHP-2088
COURSE TITLE: ORGANIC CHEMISTRY (PRACTICAL)

Course outcomes:

The students will be able to

CO1: understand and perform multi step organic synthesis.

CO2: CO2: characterize organic molecules by physical and spectroscopic methods like M.P, B.P, and IR

CO3: design multistep synthesis

CO4: expertise the various techniques of analysis of organic substances

Master of Science (Chemistry)
(Semester-II)
Session: 2022-24
COURSE CODE: MCHP-2088
COURSE TITLE: ORGANIC CHEMISTRY (PRACTICAL)

Time: 6Hrs
Credit (L-T-P): 0-0-3

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

Multistep Organic Synthesis

1. Synthesis of 2-chloro-4-bromoaniline from aniline (Bromination and chlorination) Book 1, page 292.
2. Synthesis of methyl orange from aniline.
(Aromatic electrophilic substitution and diazocoupling). Book 2, page 250.
3. Synthesis of benzpinacol and its pinacol rearrangement.
4. Synthesis of o-chlorobenzoic acid from phthalimide. Synthesis of acridone from o-chlorobenzoic acid. (Hofmann bromamide and Sandmeyer's reaction).
5. Synthesis of 2,4-dinitrophenyl hydrazine from chloro benzene. (Electrophilic and nucleophilic substitution reactions on aromatic ring).
6. Synthesis of triphenylcarbinol from bromobenzene. (Grignard reaction) Book 2, page 220.

B: Quantitative Analysis of Organic Compounds:

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

Books Recommended:

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.
2. Introduction to Organic Laboratory Techniques – A Contemporary Approach. D. L. Pavia, G. M. Lampman 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: 2022-24
COURSE CODE: MCHP-2089
COURSE TITLE: Physical Chemistry (Practical)

Course outcomes:

Students will be able to

CO1: know about the safety requirements and lab skills required to perform physico-chemical experiments

CO2: know the principle and mechanism of Conductometric and pH metric titrations experiments

CO3: study distribution of benzoic acid in organic and aqueous solvent

CO4: determine specific and molar refraction using Abbe's refractometer.

Master of Science (Chemistry)
(Semester-II)
Session: 2022-24
COURSE CODE: MCHP-2089
COURSE TITLE: Physical Chemistry (Practical)

Time: 6Hrs

Max. Marks: 75

Credit (L-T-P): 0-0-3
15)

(P: 60, CA:

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 pH metrically.
- 2) To determine dissociation constant of given acid pH metrically
- 3) Titration of weak acid conductometrically
- 4) Titration of strong acid conductometrically
- 5) To determine dissociation constant of given acid conductometrically
- 6) Determine the dissociation constant of acetic acid in DMSO, DMF, dioxane by titrating it with KOH.
- 7) Determine the activity coefficient of an electrolyte at different molalities by e.m.f. measurements.
- 8) Compare the cleansing powers of samples of two detergents from surface tension measurements.
- 9) Determine the specific refraction, molar refraction and atomic parachor with the help of Abbe's refractometer.
- 10) To study the distribution of benzoic acid between benzene and water.
- 11) Determine the equilibrium constant of reaction $\text{KI} + \text{I}_2 \rightleftharpoons \text{KI}_3$ by distribution law and hence find the value of $\log K$ of the above reaction.
- 12) Compare the relative strength of CH_3COOH and ClCH_2COOH from conductance measurements.
- 13) Determine the solubility (g/litre) of sparingly soluble lead sulphate from conductance measurements.
- 14) Titrate a given mixture of HCl and CH_3COOH against NaOH solution conductometrically.
- 15) Compare the relative strength of:
i) HCl and ii) H_2SO_4 by following the kinetics of inversion of cane sugar Polarimetrically.

Books Recommended:

1. Yadav, J. B (2005): *Advanced Practical Physical Chemistry*, 22nd 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.