FACULTY OF SCIENCES

SYLLABUS
of
M. Sc. Chemistry (Semester: I-II)

(Under Continuous Evaluation System)

Session: 2018-19

The Heritage Institution

KANYA MAHA VIDYALAYA
JALANDHAR
(Autonomous)

Scheme of Studies and Examination
M.Sc. (Chemistry)

M.Sc. (Chemistry) Semester I							
Course Code	**Course Name**	**Course Type**	**Marks**				**Examination time (in Hours)**
			Total	**Ext.**		**CA**	
				L	**P**		
MCHL-1081	Ligand Field Theory	C	50	40	-	10	3
MCHL-1082	Organic Reaction Mechanism-I	C	50	40	-	10	3
MCHL-1083	Physical Chemistry – Thermodynamics	C	50	40	-	10	3
MCHL-1084	Spectroscopy A: Techniques for Structure Elucidation of Organic Compounds	C	75	60	-	15	3
MCHM-1135	Computer for Chemists – Theory Computer for Chemists - Practical	C	75	40	20	15	3
MCHP-1086	Inorganic Chemistry Practical(Quantitative Analysis)	C	75	-	60	15	3*2
MCHP-1087	Organic Chemistry Practical	C	75	-	60	15	3*2
Total			**450**				

M.Sc Chemistry (Semester-I)
COURSE CODE: MCHL-1081
Ligand Field Theory
(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 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. 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

2. Molecular Orbital Theory for Metal Complexes:

Recapitulaltions, ligands symmetry orbitals and metal orbitals involved in molecular orbitals formation in octahderal complexes, MOEL diagrams for octahedral tetrahedral and square planar complexes showing σ and π bonding in transition metal complexes.

3. 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

4. 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

5. 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, elecronic delocalization, magnetic properties of d^n and f^n metal ions.

UNIT-IV

6. Electronic Spectra of Transition Metal Complexes:

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^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$[Co(en)_2X_2]^+$, $[Mn(H_2O)_6]^{2+}$, $CuSO_4.5H2O$ and its anhydrous complex, comparison of d–d band with f–f bands. Introduction to Charge Transfer Spectra.

Recommended Books:

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.

Time: 3 hrs   **Max. Marks: 50**
                                                    (Theory: 40, CA: 10)

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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

1. Nature of Bonding in Organic Reactions:

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

2. 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

3. 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.

4. Aliphatic Nucleophilic Substitution – A:

The SN2, SN1 and SNi mechanisms, mixed SN1 & SN2 mechanism SET mechanism. The neighbouring group mechanism (anchimeric assistance). Neighbouring group participation by pi and sigma bonds.

UNIT-III

5. 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.

6. 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 sulphur ylides, effect of substrates, leaving group and solvent polarity on the reactivity.

UNIT-IV

7. 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.

8.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.

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

(Session-2018-19)
M.Sc Chemistry (Semester-I)
COURSE CODE: MCHL-1083
Physical Chemistry – Thermodynamics
(Theory)

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

Time: 3 Hrs.

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

1. 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

2.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.

3.Statistical Thermodynamics:
Concept of distribution law, thermodynamic probability and most probable distribution, Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical 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.

3. 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.

Books Suggested:

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. Lee Bot

4.   I Prigogine: Introduction to thermodynamics of irreversible processes

5.   T L Hill: Introduction to statistical thermodynamics.

M.Sc Chemistry (Semester-I)
COURSE CODE: MCHL-1084
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 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. Nuclear Magnetic Resonance
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 tyupical chemical Shifts simple application of chemical shifts, ring current and aromaticity. Shifts for H and ^{13}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

2. 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, Reteroiels – Alder fragmentation. Cleavage associated with common functional groups (Aldehydes, ketones cyclic and acyclic esters, alcohols, lefins, aromatic compounds amines). - Special methods of GCMS, high resolution MS, Introduction to radical anion mass spectroscopy. Interpretation of the spectrum of an unknown.

3. Ultraviolet and Visible Spectroscopy
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

4. 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 & conformational analysis.
(f) Studying reactive species

UNIT-IV

5. Solution of Structural Problems by Combined Use of the following Spectroscopic Techniques:
(a) Electronic spectra
(b) Vibrational spectroscopy
(c) NMR (^{1}H and ^{13}C) 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 & G.C. Bassler, Spectrometric Identification of Organic Compounds.

5. R.C. Banks, E.R. Matjeha and G. Mercer, Introductory Problems in Spectroscopy.

6. Introduction to Spectroscopy - Pavia

(Session-2018-19)
M.Sc Chemistry (Semester-I)
COURSE CODE: MCHM-1135
Computer for Chemists

Time: (3+3) hrs.

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 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.

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 quardratic 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 wave length.
7. Calculation of van der Waals radii.
8. Radioactive decay.
9. Rate constant of a 1st order reaction, 2nd order reaction.
10. Determination
11. Calculation of lattice energy using Born Lande equation.

UNIT-III
12. Addition, multiplication and solution of inverse of 3 X 3 matrix.
13. Calculation of average molecular weight of a polymer containing n1 molecules of molecular weight m1, n2 molecules of molecular weight M2 and so on.
14. Program for calculation of molecular weight of organic compound containing C, H, N, O and S.
15. Calculation of reduced mass of diatomic molecule.
16. Calculate the RMS and most probable velocity of a gas.

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

Recommended Books:
1. K.V. Raman, Computers in Chemistry, Tata McGraw Hill.
2. Mullish Cooper, The spirit of c, An Introduction to Modern Programming.

Time: 60 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-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^{-1} and $C_2O_4^{-2}$ ions.

3. Standardization of $K_2Cr_2O_7$ with Fe^{2+} and determination of Fe^{3+} (Ferric alum)

4. Standardization of hypo solution with potassium iodate / $K_2Cr_2O_7$ 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.

Book: Vogel's book on Inorganic 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.

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 tea leaves*
   (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 reactions proteins).

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, methyl 3-nitrobenzoate.

5. *Cannizaro'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 chlorobenzadehyde, 4-chlorobenzoic acid 4-chlorobenzyl alcohol.

6. *Synthesis of 1,3,5-Tribromobenzene from aniline*. **Aim:** To demonstrate: Bromination, Diazotization and Reduction.

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

Course Code	Course Name	Course Type	Marks				Examination time (in Hours)
			Total	Ext.		CA	
				L	P		
MCHL-2081	Organometallics Chemistry	C	50	40	-	10	3
MCHL-2082	Organic Reaction Mechanism -II	C	50	40	-	10	3
MCHL-2083	Physical Chemistry – Quantum Chemistry	C	50	40	-	10	3
MCHL-2084	Reaction Mechanisms and Metal clusters	C	50	40	-	10	3
MCHL-2085	Spectroscopy B: Techniques for Structure Elucidation of Inorganic Compounds	C	75	60	-	15	3
MCHL-2336 MCHL-2057	Mathematics for Chemists Or Biology for Chemists	C	25	20	-	5	2
MCHP-2088	Organic Chemistry Practical	C	75	--	60	15	3*2
MCHP-2089	Physical Chemistry Practical	C	75	--	60	15	3*2
Total			**450**				

M.Sc. (Chemistry) Semester II

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:

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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. η^2- ligands: olefenic and acetylenic complexes, chelating olefenic 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 cyclopentdienyl complex, Preparation of cyclopentadieny T.M. Complexes. MO treatment of ferrocene. η^6 – ligands: Benzene and its derivatives. Multidecker sandwich compounds.

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

π-acid ligands (15 Hrs.)

π- acceptor character of CO, O_2, N_2, NO, PH_3 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; tertiaryohosphine as ligand.

Books Recommended:

1. C. Elschenbroich and A. Salzer, Organometallics: A Concise Introduction, 2nd Ed., 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 & VI.WileyInter-science.

4. G. L. Miessler, D. A. Tarr, Inorganic Chemistry, 3rd edition, Pearson Education

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

Time: 3 hrs.

Instructions for the Paper Setters:

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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 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, 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. Base-catalyzed 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 centre reactions. Diels-Alder reaction, 1-3 Dipolar additions.

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

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

Time: 3 hrs.

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

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

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

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 cyclo propenyl 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.

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 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

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 carbonyl scrambling.

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.

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 carboranes metallocarboranes, 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.

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 & Wilkinson: Inorganic Chemistry V & VI Ed. Willy Eastern – (1999).

4.   J.E. Huheey: Inorganic Chemistry III & IV Ed. Pearson Education Asia – (2002).

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

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

Time: 3 hrs.

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

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, force constant.
- 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 vibration concepts.
- 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, 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).

UNIT-III
(A)

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

(i) Metal carbonyls.

(ii) NSF_3

(iii) Geometrical isomerisan – differentiation between Cis and trans. $[Co(bipy)_2Cl_2]Cl$.

(iv) Structures of $CO2$, $N2O$, $H2O$, chlorocomplexes of mercury, camium and zinc and some octahedral complexes $ML6$ (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+}, Zu^{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 & 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 lattiee on the magnitude of eQ4, double resonance technique, Application ($PFCl_4.PCl_5$), $(NH_4)_2TeCl_6$, , group 14 tetra halides, R_3MX_2 (M=As,Sb,Bi), Cis & Trans$[Co(en)_2Cl_2]Cl$, 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 {$^{57}F_e$, $^{119}S_N$, $^{151}E_U$ compounds, to biological systems to surface study, I_2Cl_6, $IBr_2 Cl_4$, XeF_4, $XeCl_4$.

Books Recommended:

1. E.A.V Ebsworth; W.H Renkin; Cradock, Structure Methods in Inorganic Chemistry.
2. R.S Drago, Physical Methods for Chemists (Ist and IInd Edition).
3. C.N Banwell, Fundamentals of Molecular Spectroscopy.
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, Mossbauer Spectroscopy.
7. K. Nakamoto, Infrared Spectra of Inorganic and co-ordination Compounds.

MATHEMATICS FOR CHEMISTS
(For Medical Students)

Course Outcomes

After the successful completion of this subject, the students should be able to:

CO 1: Understand the trigonometric functions with the help of unit circle and application of trigonometric identities.

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 of system of linear equations.

CO 3: Understand the concept of Eigen vectors and Eigen values of matrices.

CO 4: 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 5: Recognize Integration as an inverse of differentiation and to calculate area under curve and understand integrals as limit of sum and its geometrical interpretation.

(Session-2018-19)
M.Sc Chemistry (Semester-II)
COURSE CODE: MCHL-2336

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 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 ofmatrices.

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 implict 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.

Books Recommended:

1. Santi Narayan & P.K. Mittal – Differential Calculus.

2. Santi Narayan & P.K. Mittal - Integral Calculus.

3. B.S. Grewal – Higher Engineering Mathematics.

4. Joseph B. Dence – Mathematical Techniques in Chemistry.

5. Margenau and Murphy, the Mathematics of Physics   and Chemistry.

6. B.L. Moncha and H.R. Choudhary – A Text Book of Engineering Mathematics.

BIOLOGY FOR CHEMISTS
(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 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

The Organisation of Life
1. Biologically important molecules: Carbohydrates, lipids, proteins and nucleic acids.
2. The life of cells – The cell theory, general characteristics of cells, difference between prokaryotic and eukaryotic cells, difference between plant and animal cells, cell organells.

UNIT-II

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

UNIT-III

Genetics

4. The basic principle of heredity: Mendals law, monohybrid cross, dihybrid cross.
5. DNA – Double halix structure and replication.
6. Genes expression: Transcription and translation, genetic code.

UNIT-IV

The Diversity of Life

7. The classification of Living things – Criteria of classification, Whittaker's systems of classification, their characteristics with are example of each.
8. Viruses, structure of Viruses.

Book Recommended:

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

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

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 fromo-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, Ranehart and Winston Inc. New York.

2. 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.

(Session-2018-19)
M.Sc Chemistry (Semester-II)
COURSE CODE: MCHP-2089
Physical Chemistry (Practical)

Time: 60 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 $_P$H 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 Kl +l2 $\rightarrow$ Kl3 by distribution law and hence find the value of go of the above reaction.
12) Compare the relative strength of CH_3COOH and $CICH_2COOH$ 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.