

DR. BABASAHEB AMBEDKAR MARATHWADA
UNIVERSITY,
AURANGABAD.

DEPARTMENT OF CHEMISTRY



SYLLABUS

M. Sc. Chemistry

(Semester I to IV)

Choice Based Credit and Grading System

Effective from : June 2016

Structure and Curriculum for M. Sc. Chemistry programme (Choice Based Credit and Grading System)

The M. Sc. Chemistry programme is divided into four semesters having 108 credits. There are 19 theory courses of 63 credits, 09 laboratory courses of 27 credits, research project of 18 credits (distributed in IV semester) and one course is on constitution of India is of 02 credit. Tutorials, assignments and seminar presentation are integral component of all theory courses. Approximately, 44% are of core courses, 4% foundation courses, and 7% are elective courses, 25% laboratory courses and 20% research project.

Eligibility:

Those who have completed B. Sc. with Chemistry as an optional subject from any recognized University/ Institution are eligible for registration subject to the rules and regulations laid down by Dr. Babasaheb Ambedkar Marathwada University, Aurangabad.

Admission / Promotion Process:

In response to the advertisement for registration, interested students will have to register themselves. Admission will be done on the basis of Common Entrance Test (CET) (50% weightage) and performance of students at their qualifying graduate level examination (50% weightage of Marks obtained in the subject of Chemistry at B. Sc level). Once the student is admitted he/she will be promoted to the 2nd year (3rd semester) as per university rules and regulations. The admission of the concern student will be automatically cancelled if he / she fails to complete the M. Sc. degree within a period of maximum four years / eight semesters.

Choice Based Credit System (CBCS) :

The choice based credit system has been adopted by this department. This provides flexibility to make the system more responsive to the changing needs of our students, the professionals and society. It gives greater freedom to students to determine their own pace of study. The credit based system also facilitates the transfer of credits.

Credit-to- contact hour Mapping:

One contact hour per week is assigned 1 credit for theory and 0.5 credits for laboratory courses/ research project. Thus a 4- credit theory course corresponds to 4 contact hours per week and same analogy will be applicable for laboratory courses / research project.

Semester- I (Core and Foundation Courses)				
Paper No.	Course Title	Teaching (hrs/week)	Marks	Credits
CHEC-101	Inorganic chemistry	04	100	04
CHEC-102	Organic chemistry	04	100	04
CHEC-103	Physical chemistry	04	100	04
CHEF-104	Analytical chemistry	02	50	02
COM-100	Constitution of India	02	50	02
CHELI-105	Laboratory course	06	50	03
CHELO-106	Laboratory course	06	50	03
CHELP-107	Laboratory course	06	50	03
Total Credits for Semester I: 25 (Theory: 16; Laboratory: 09)				

Semester- II (Core and Foundation Courses)				
Paper No.	Course Title	Teaching (hrs/week)	Marks	Credits
CHEC-201	Inorganic chemistry	04	100	04
CHEC-202	Organic chemistry	04	100	04
CHEC-203	Physical chemistry	04	100	04
CHEF-204	Analytical chemistry	02	50	02
CHEF-205	Research methodology	02	50	02
CHER-206	Review of literature	01	25	01
CHELI-207	Laboratory course	06	50	03
CHELO-208	Laboratory course	06	50	03
CHELP-209	Laboratory course	06	50	03
Total Credits for Semester II: 26 (Theory: 17; Laboratory: 09)				

Semester- III (Core and Elective Courses) Inorganic Chemistry				
Paper No.	Course Title	Teaching hrs/week	Marks	Credits
CHESC-301	Structural elucidation by spectral methods	04	100	04
CHECI-302	Bioinorganic and supramolecular chemistry	04	100	04
CHECI-303	Applied inorganic chemistry	04	100	04
CHEEI-304	Chemistry of materials	04	100	04
CHEEI-305	Environmental chemistry OR	04	100	04
CHEEI-306	Solid state chemistry OR	04	100	04
CHELI-307	Laboratory course	06	50	03
CHELI-308	Laboratory course	06	50	03
CHELI-309	Laboratory course	06	50	03
Total Credits for Semester III: 25 (Theory: 16; Laboratory: 09)				

Semester- III (Core and Elective Courses) Organic Chemistry				
Paper No.	Course Title	Teaching hrs/week	Marks	Credits
CHESC-301	Structural elucidation by spectral methods	04	100	04
CHECO-302	Organic synthesis	04	100	04
CHECO-303	Pericyclic reactions, photochemistry and free radicals	04	100	04
CHEEO-304	Advanced organic chemistry	04	100	04
CHEEO-305	Environmental chemistry OR	04	100	04
CHEEO-306	Green chemistry OR	04	100	04
CHELO-307	Laboratory course	06	50	03
CHELO-308	Laboratory course	06	50	03
CHELO-309	Laboratory course	06	50	03
Total Credits for Semester III: 25 (Theory: 16; Laboratory: 09)				

Semester- III (Core and Elective Courses) Physical Chemistry				
Paper No.	Course Title	Teaching hrs/week	Marks	Credits
CHESC-301	Structural elucidation by spectral methods	04	100	04
CHECP-302	Solid state chemistry	04	100	04
CHECP-303	Thermodynamics	04	100	04
CHEEP-304	Advanced electrochemistry OR	04	100	04
CHEEP-305	Nuclear chemistry OR	04	100	04
CHEEP-306	Environmental chemistry	04	100	04
CHELP-307	Laboratory course	06	50	03
CHELP-308	Laboratory course	06	50	03
CHELP-309	Laboratory course	06	50	03
Total Credits for Semester III: 25 (Theory: 16; Laboratory: 09)				

Semester- IV (Core and Elective Courses) Inorganic Chemistry				
Paper No.	Course Title	Teaching hrs/week	Marks	Credits
CHECI-401	Nuclear chemistry	02	50	02
CHECI-402	Photoinorganic chemistry	04	100	04
CHECI-403	Therapeutic bioinorganic and forensic chemistry	04	100	04
CHEEI-404	Organo transition metal chemistry OR	04	100	04
CHEEI-405	Polymer chemistry OR	04	100	04
CHEEI-406	Theoretical and structural inorganic chemistry	04	100	04
CHEIR-407	Research project (Experimental)	24	200	12
CHEIR-408	Research project (Dissertation, presentation and Seminars)	06	100	06
Total Credits for Semester IV: 32 (Theory: 14; Laboratory: 18)				

Semester- IV (Core and Elective Courses) Organic Chemistry				
Paper No.	Course Title	Teaching hrs/week	Marks	Credits
CHECO-401	Heterocyclic chemistry	02	50	02
CHECO-402	Organic synthesis: Retrosynthetic approach	04	100	04
CHECO-403	Chemistry of natural products	04	100	04
CHEEO-404	Medicinal chemistry OR	04	100	04
CHEEO-405	Organic high polymers OR	04	100	04
CHEEO-406	Drug design and drug discovery	04	100	04
CHEOR-407	Research project (Experimental)	24	200	12
CHEOR-408	Research project (Dissertation, presentation and Seminars)	06	100	06
Total Credits for Semester IV: 32 (Theory: 14; Laboratory: 18)				

Semester- IV (Core and Elective Courses) Physical Chemistry				
Paper No.	Course Title	Teaching hrs/week	Marks	Credits
CHECP-401	Surface and magnetochemistry	02	50	02
CHECP-402	Polymer chemistry	04	100	04
CHECP-403	Chemical dynamics and catalysis	04	100	04
CHEEP-404	Nanochemistry OR	04	100	04
CHEEP-405	Quantum chemistry OR	04	100	04
CHEEP-406	Biophysical chemistry	04	100	04
CHEPR-407	Research Project-3(Experimental)	24	100	12
CHEPR-408	Research project (Dissertation, presentation and Seminars)	06	50	06
Total Credits for Semester IV: 32 (Theory: 14; Laboratory: 18)				

CHEC-101: Inorganic Chemistry

04 Hrs/Week

Credits: 04

Marks : 100

Unit-I: Group theory and Symmetry concepts

12 hrs

Symmetry elements and symmetry operations, Center of symmetry(i), Axis of symmetry (C_n), Plane of symmetry (σ_v , σ_h , σ_d), Rotation reflection axis of symmetry(S_n), Identity(E). point groups, classifications of point groups, Identification of point group of : H_2O , NH_3 , CO_2 , BF_3 , C_2H_4 , PCl_3 , PCl_5 , $[PtCl_4]^-$, cis and trans $[PtCl_2(NH_3)_2]$, $[CoCl_2(NH_3)_4]$, $[FeF_6]$, H_2 , HCl , CO , BeF_2 , $C_2H_2Cl_2$, C_6H_6 , and substituted benzene molecule. Application of point group with respect to dipole moment, polar and non polar molecules, definition of group, properties of group.

Unit-II: Representations of groups

12 hrs

Group multiplication tables, matrix representation of symmetry elements. Reducible and irreducible representation, character of representation, character of matrix, Conjugate matrix, Properties of irreducible representations, Great orthogonality theorem (without proof) and it's importance, construction of character table of C_{2v} & C_{3v} point group. Mulliken symbolism rules for irreducible representations. Standard reduction formula, direct product and uses.

Unit-III : Reaction mechanism of transition metal complexes.

12 hrs

Classification of inorganic reactions, ligand substitution reaction and their mechanisms of octahedral complexes. Acid hydrolysis, factors affecting the acid hydrolysis. Base hydrolysis, conjugate base mechanism. Electron transfer reaction: mechanism of inner and outer sphere electron transfer reactions in octahedral complexes.

Unit-IV: Metal ligand equilibria in solution:

12 hrs

Definition of stability constant, step wise and overall formation constant, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand. Determination of formation constant for binary complexes using pH-metric technique.

Unit-V: Inorganic chemistry in biological systems

12 hrs

Essential and trace elements in biological systems and their functions , structure and function of metalloporphyrins, Hemoglobin, cytochrome and hemocyanine. Electron transfer, Respiration and photosynthesis reaction, Metal deficient diseases of Fe, Zn, Cu and Mn and their therapy.

Reference books:

1. Concise Inorganic Chemistry, J.D.Lee.
2. Inorganic Chemistry, J.E.Huhey and Keiter R. L
3. Symmetry and Spectroscopy of Molecules, K.Veera Reddy.
4. Group Theory and symmetry in Chemistry, Gurdeep Raj.Ajay Bhagi and Vinod Jain.
5. Symmetry and Group theory in Chemistry , R Ameta
6. Mechanism of Inorganic Reaction. II Edn. Fred Basolo and R.G.Pearsons.
7. Selected Topic in Inorganic Chemistry, Wahid U. Malik, G.D.Tuli and R.D.Madan.
8. Advanced Inorganic Chemistry, F.A.Cotton and Wilkinson.
9. Advanced Inorganic Chemistry, Satyaprakash, G.D.Tuli, S.K.Basu and R.D.Madan.
10. Advanced Inorganic Chemistry, Volume I and II Gurdeep Raj.
11. A Textbook of bioinorganic chemistry, A. K. Das

--

-

CHEC-102: Organic Chemistry

04 Hrs/Week

Credits: 04

Marks : 100

Unit-I: Nature of Bonding in Organic Molecules

12 hrs

Delocalized chemical bonding, conjugation, cross conjugation, resonance, hyperconjugation, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant compounds, Huckel rule, energy level of π -molecular orbitals, annulenes, aromaticity, Bonds weaker than covalent - addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

Unit-II: Reaction Mechanism : Structure and Reactivity

12 hrs

Types of Mechanisms, Types of reactions, Thermodynamic and Kinetic requirements, Kinetic and Thermodynamic control, Hammond's postulate, methods of determining mechanisms, isotope effects.

Generation, structure, stability and reactivity of carbocations, Carbanions, free radicals, carbenes and Nitrenes. Effect of structure on reactivity, resonance and field effect, steric effect quantitative treatment, The Hammett equation, Linear free energy relationship, substituent and reaction constants, Taft equation.

Unit-III & IV: Stereo-chemistry

24 hrs

Elements of symmetry, chirality, Enantiomeric and diastereomeric relationships, R and S, E and Z nomenclature. Molecules with more than one chiral center, Threo and Erythro isomers, Prochiral relationships, groups and faces, stereospecific and stereoselective reactions. Optical activity in the absence of Chiral Carbon (Biphenyls, allenes and Spiranes), Chirality due to helical shape. Methods of resolution, optical purity, stereochemistry of the compounds containing Nitrogen, Sulphur and phosphorous. Conformational analysis of cycloalkanes, Mono and disubstituted cyclohexanes, decalins, effect of conformation on reactivity

Unit-V: Aliphatic Nucleophilic Substitutions

12 hrs

Nucleophilic: The S_{N}^2 , S_{N}^1 mixed S_{N}^1 and S_{N}^2 and SET mechanisms. The neighbouring group mechanism, Neighbouring group participation by π and σ -bonds, anchimeric assistance. Nucleophilic Substitution at an allylic aliphatic trigonal and a vinylic carbon.

Reactivity: Effect of substrate structure, attacking nucleophile, leaving group and reaction medium. Phase transfer catalysis, Ambident nucleophiles, regioselectivity.

Reference Books:

1. Advanced Organic Chemistry, IV Edition: J. March
2. Stereochemistry of Carbon Compounds: E. L. Eliel
3. Advanced organic Chemistry, Part-A and Part-B: F. A. Carey, & R. J. Sundburg.
4. A Guide Book to Mechanisum in Organic Chemistry: Peter Sykes.
5. Principles of Organic Synthesis: R. O. C. Norman
6. Stereochemistry of Organic Compounds: D. Nashipuri
7. Organic Chemistry: Clayden and Greeves
8. Mechanism and Structure in Organic Chemistry: E. S. Gould

Unit-I: Ionic Equilibria and Biological Reactions**12 hrs**

Exact treatment of the dissociation of weak acids and bases, Dissociation constant of polyprotic acids, Statistical effects in polyprotic acids, Dissociation constant of complex ions, Logarithmic expression for pH and pOH, Calculations involving buffer solution, buffer capacity and buffer index, Salt effect and solubility product and its applications.

Thermodynamics of biochemical reactions, Binding of oxygen by myoglobin and hemoglobin, Reaction between microscopic and macroscopic dissociation constant.

Unit-II: Chemical Dynamics**12 hrs**

Collision theory, modified collision theory, weakness of the collision theory, Theory of absolute reaction rates, equilibrium hypothesis, Derivation of the rate equation, statistical mechanical derivation and thermodynamic formulation. Isotope effect on reaction rate. Primary salt effect, secondary salt effect.

Dynamics of uni-molecular reactions, Lindmann and Hinshelwood theory

Kinetics of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and NMR method.

Reactions in solution: Reaction between ions, influence of solvent-double sphere model, single sphere model, influence of ionic strength, numericals.

Unit-III: Classical Thermodynamics**12 hrs**

Nernst heat theorem, the third law of thermodynamics, determination of absolute entropies of solids, liquids and gases. Partial molar properties : Partial molar free energy, chemical potential, partial molar volume and partial molar heat content and their significance, determination of these quantities, concept of fugacity and determination of fugacity.

Unit-IV: Surface Chemistry:**12 hrs**

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

Colloidal electrolytes, Types of micelles in colloidal electrolytes, Micellization, Thermodynamics of micellization, Mechanism of Micellization, critical micellar concentration, Determinations of critical micellar concentration, Surface active agents, Classifications of surface active agents, Reverse micelles, Solubilization

Unit-V: Electro-Chemistry**12 hrs**

Debye-Huckel theory of strong electrolytes, Debye-Huckel-Onsager equation Testing of the equation, Debye-Falkenhagen effect, Wein effect, activity coefficient, mean ionic activity coefficient; Debye-Huckel limiting law ionic strength. Electrocapillary phenomena, and its measurements. Effect of anions, cations and molecules on electrocapillary curves. Electrocapillary properties of mercury-solution interface.

Polarography: the Ilkovic equation and its derivation, concentration polarization, instrumentation, advantages of DME, half wave potential. Applications of polarography, numerical.

References books:

1. Chemical Kinetics - Laidler (McGraw-Hill)
2. Kinetic and Mechanism of Chemical Transformations - J. Rajaram and J.C. CURIACOSE (Macmillan India Ltd.)
3. Physical Chemistry - Atkins (Oxford)
4. Thermodynamics for Chemists - S. Glasstone (EWP, New Delhi)
5. Physical Chemistry - G. M. Barrow
6. Advanced Physical Chemistry - Gurdeep-Raj (Pelenum)
7. Micelles : Theoretical and Applied Aspects - V. Moroi (Plenum)
8. Text Book of Physical Chemistry - S.Glasstone (McMillan)
9. An Introduction to Electrochemistry - S. Glasstone (EWP, New Delhi)
10. Physical chemistry – Robert A .Alberty ., Robert J .Silbey
11. Statistical Thermodynamic – M. C. Gupta

CHEF-104 : Analytical Chemistry

02 Hrs/Week

Credits: 02

Marks : 50

Unit-I: Basic concepts of analytical chemistry:

15 hrs

The role of analytical chemistry, qualitative and quantitative analysis, The analytical process, Validation of a method.

Statistical treatment of analytical data:

Introduction, types of errors, significant figures, precision and accuracy, methods of expressing accuracy, methods of expressing precision, the confidence limit, tests of significance- the F test, the student T test, rejection of results - the Q test. Statistics for small data sets, linear least squares, correlation coefficient, using spreadsheets for plotting calibration curves, slope, intercept and coefficient of determination, numericals.

Unit-II: Basic separation techniques:

15 hrs

Distillation and solvent and solid phase extraction:

Distillation: Fractional distillation, distillation under vacuum, theory of operation of distillation methods, some practical considerations.

Solvent and Solid Phase extraction: Phase equilibrium, the partition coefficient the distribution ratio, theory of phase contact methods, single equilibrations, repeated equilibrations, counter current distribution, practical aspects and applications - extraction of metals, extraction of molecular species, Ion pair extractions, Accelerated and microwave assisted extraction, solid phase extraction, Numericals.

Chromatography

Introduction, basic principles and theory of chromatographic techniques, plate theory of chromatography, rate theory of chromatography, other factors in zone broadening, Development of the chromatogram - Frontal analysis, elution analysis displacement analysis, selection of chromatograph system, qualitative and quantitative analysis by chromatography.

Reference Books:

1. Fundamental of Analytical Chemistry 8th Edⁿ. Skoog, West Hollar, Couch.
2. Analytical Chemistry 6th Edition., Gary D. Christian
3. Chemical Separations and Measurements, D.G. Peters, J.M. Hayes and G.M. Hieftie
4. Instrumental Method of Chemical Analysis, G.R. Chatwal & S.K. Anand.

COM - 100 : Constitution of India

02 Hrs/Week

Credits: 02

Marks : 50

—

--

CHELI -105 : Laboratory Course

06 Hrs/Week

Credits: 03

Marks : 50

List of experiments

I. Preparation and estimation of percentage metal ion present in a metal complexes.

- | | | |
|---|---|--|
| 1. $\text{Ti}(\text{C}_9\text{H}_8\text{NO})_2 \cdot 2\text{H}_2\text{O}$ | 2. $\text{VO}(\text{acac})_2$ | 3. $\text{Cis-K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$ |
| 4. $[\text{Mn}(\text{acac})_3]$ | 5. $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]$ | 6. $\text{Hg}[(\text{Co}(\text{SCN})_4)]$ |
| 7. $[\text{Co}(\text{III})(\text{NH}_3)_6]\text{Cl}_3$ | 8. $[\text{Co}(\text{III})(\text{NO}_2)(\text{NH}_3)_5]\text{Cl}_2$ | 9. $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$ |

II. Separation and estimation of amount of metal ions from the following mixture solutions

1. Copper- Nickel
2. Nickel- Zinc
3. Iron- Magnesium

Reference Book:

1. A Text book of Quantitative Inorganic Analysis; A. I. Vogel
2. Practical Inorganic Chemistry; Pass Geoffrey and Haydn Sutcliffe.
3. Advanced Practical Inorganic Chemistry; Gurudeep Raj;.
4. Vogel's Qualitative Inorganic Analysis, D. Svehla, VII Edn. Orient Longman Ltd.

Scheme of Marking

Preparation & estimation of percentage of metal ion Metal Complexes 25 Marks

- | | |
|---|----------|
| i). Yield of complexes | 15 Marks |
| ii). Observation table, Calculation & Results | 10 Marks |

II. Separation and Estimations of binary mixture of metal ions: 15 Marks

- | | |
|----------------------------|----------|
| i). Observation table | 05 Marks |
| ii). Calculation & Results | 10 Marks |

III. Journal and Viva-Voce 10 Marks

--

CHELO- 106: Laboratory course

06 Hrs/Week

Credits: 03

Marks: 50

List of experiments

1. Qualitative Organic Analysis: Marks: 25

Separation, purification and identification of binary (**Solid-Solid**) mixtures.

The separation should be carried out using Chemical method.

The two components are solid-solid mixtures.

Student should submit the purified samples of the separated compounds and prepare a suitable derivative of the two compounds separated out.

Note : Analysis of at least five mixtures should be carried out.

2. Single Stage Preparations: Marks: 15

i) *p*-nitro acetanilide from acetanilide.

ii) Dibenzylidene acetone from Benzaldehyde

Note: i) The preparations should be carried out using (0.02 to 0.05 mole) of the starting material.

ii) The yield, melting point and TLC of the recrystallised product should be recorded.

Note : Student will not be allowed for practical examination if his/her record book is not completed and certified.

3. Record Book & Viva Marks: 10

Scheme of Marking:

1. Qualitative Organic Analysis (Analysis of one Component is Compulsory)

Marks

i) Type of the mixture	07
ii) Preliminary test	02

Analysis of the individual components:

iii). Detection of Elements	03
iv) Detection of functional groups	03
v) Determination of MP/BP	04
vi) Preparation of the derivative	04
vii) Identification (Spotting)	02

2. Preparation

i) Brief experimental procedure along with mechanism and calculations	05
ii) Submission of recrystallized product	05
iii) Yield and MP of pure product	05

List of experiments
A. Instrumentation.

1. Determination of strengths of halides in a mixture potentiometrically.
2. Determination of the strength of strong and weak acid in a given mixture conductometrically.
3. Determination of solubility and solubility product of sparingly soluble salt BaSO_4 .
4. Determine the pK_1 and pK_2 value of phosphoric acid by pH metry.
5. Determine the indicator constant of given indicator by colorimetric measurements.
6. Study of kinetics of inversion of cane sugar.

B. Non-Instrumentation.

1. Determine the molecular refraction of methyl acetate, ethyl acetate, n-hexane and carbon tetrachloride and calculate the refraction of CH_2 , C, H and O atoms.
2. To study the effect of surfactants (sodium chloride) on surface tension of given liquid.
3. To determine the radius of molecule by viscosity measurements.
4. Determine the solubility of benzoic acid in water at different temperature and hence its heat of solution.
5. Determine the formula of the complex formed between Cu(II) and ammonia by distribution method.
6. Determine the velocity constant of hydrolysis of ester.

Note : Student will not be allowed for practical examination if his/her record book is not completed and certified.

Reference Book

1. Systematic experimental physical chemistry – T. K. Chondhekar & S.W. Rajbhoj
2. Experiments in chemistry – D.V. Jahagirdar

Scheme of marking :

1) Experiment I (Instrumentation)	Experiment -II (Non-instrumentation)
Max .Marks	Max. Marks
i) Observation :	08
ii) Calculation :	04
iii) Graph :	04
Accuracy& Results :	04
Record book & Viva :	05

Unit-I : Spectroscopic term symbols**12 hrs**

Terms, Inter-electronics repulsion, spin orbit coupling, ground terms, determination of terms symbol of d^1 to d^5 Configuration / complexes, Energy ordering of terms, microstates. Racah parameter. Weak and stronger field approach. Correlation diagram of d^1 , d^2 , d^8 and d^9 configuration in octahedral and tetrahedral environments, Non-crossing rule. Orgel diagram of d^1 to d^9 configuration in an octahedral and tetrahedral environments, Tanabe Sugano diagram of d^2 and d^3 configurations.

Unit-II: Interpretation electronic Spectra of metal complexes**12 hrs**

Experimental measurement of the spectra, Charge transfer transitions, types of charge transfer transitions, Band intensities, intensity of d-d bands and charge transfer bands. Interpretation of electronic spectrum of transition metal complex with suitable examples. Konig's method for calculation of D_q , B and β parameters and numericals.

Unit-III: Chemistry of Metal Carbonyls**12 hrs**

Classification; Chemistry of carbonyl group Preparation, properties, structures and bonding in - iron carbonyls, $Ni(CO)_4$, $Co_2(CO)_8$, $Mn_2(CO)_{10}$, $Cr(CO)_6$, $Mo(CO)_6$ and $W(CO)_6$, $Co_4(CO)_{12}$ and $V(CO)_6$. EAN rule applied to these carbonyls structures of mixed carbonyls of transition metals and EAN rule applied to these carbonyls. Preparations carbonyl halides

Unit-IV: Metal nitrosyl compounds**12hrs**

Preparations and properties of Nitrosyl halides (NOX), Metal nitrosyl halides, compounds containing NO- group, Compounds containing NO^+ groups, Preparation, structure and application of sodium Nitropruside. EAN and Eighteen electron rules applied to: Nitrosyl compounds of Cobalt, iron and Manganese. Significance of NO for the life of living animal

Unit-V: Chemistry of dioxygen, dinitrogen complexes and non-carbonyl**metal clusters****12 hrs**

A. Preparation structure and function of Cobalt dioxygen complexes.

Preparation, properties, structures and function of dinitrogen complexes of Molybdenum, Structures and function of nitrogenase enzymes .

B. Preparation, structure and bonding in Non-carbonyl metal clusters viz. Binuclear $(Re_2Cl_9)^{2-}$, Trinuclear $(ReCl_3)_3$, Tetranuclear $(W_4(OR)_6)$ and Hexanuclear $(Mo_6Cl_6)^{4+}$ ions. Preparation , properties and structures of Zintl anions & cation of Ge, Sn, and Bi

References Books:

1. Inorganic Chemistry , J.E. Hubeey, E.A. Keitler, R.L. Keitler.
2. Concise Inorganic Chemistry - J.D. Lee.
3. Inorganic electronic spectroscopy, - A.B.P. Lever.
4. Symmetry and Spectroscopy of Molecules - K. Veera Reddy
5. Symmetry and Group theory in Chemistry , R Ameta
6. Inorganic Chemistry (IIIrd Edition) - G.Y. Miessler and D.A. Tarr.
7. Advanced Inorganic Chemistry - Vol. I - Satyaprakash, Tuli, Basu and Madan.
8. Selected Topics in Inorganic Chemistry - W.U. Malik, G.D. Tuli & R.D. Madan.
9. Chemistry of the Elements - N. N. Greenwood and A. Earnshaw.
10. Inorganic Chemistry - Attkin and Shriver.
11. Advanced Inorganic Chemistry Vol. I & Vol. II - Gurdeep and Raj.
12. Some aspect of Crystal Field theory- T. M. Dunn, D.S.Mcclure & R. G. Person

-

--

Unit-I: Aromatic Electrophilic and Nucleophilic Substitutions**18 hrs**

Electrophilic Substitutions: The arenium ion mechanism, orientation and reactivity, energy profile diagram. The ortho/para ratio, IPSO substitution, orientation in other ring system, Recapitulation of halogenation, nitration, sulphonation and Friedel Craft's reaction, diazonium coupling.

Nucleophilic Substitution: The SN^{Ar} , SN^1 , benzyne mechanism, Effect of substrate structure, leaving group and attacking nucleophile on reactivity.

Unit-II: Addition to Carbon –Carbon multiple bond:**12 hrs**

Mechanism and stereochemical aspect of addition reaction involving electrophile, nucleophile and free radicals. Regioselectivity and chemoselectivity, orientation and reactivity, Michael addition, Sharpless asymmetric epoxidation.

Unit-III: Addition to Carbon–Hetero Multiple bond:**12 hrs**

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acid, ester and nitriles. Addition of Grignard reagent, Organo zinc and organo lithium reagent to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation reaction involving enolates –Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin, Stobbe reaction. Hydrolysis of esters.

Unit-IV: Elimination Reactions:**12 hrs**

The E_1 , E_2 , and E_{1CB} mechanism, orientation of double bond. Reactivity: effect of substrate structure, attacking base, the leaving group and the medium, pyrolytic elimination.

Unit-V: Rearrangements:**06 hrs**

General mechanistic consideration, nature of migration, migratory aptitude, memory effect, pinacol-pinacolone, Benzil–Benzilic acid, Beckmann, Hoffman and Fries rearrangements.

Reference Books:

1. Advanced Organic Chemistry, IV Edition: J. March
2. Advanced organic Chemistry, Part-A and Part-B: F. A. Carey, & R. J. Sundburg.
3. A Guide Book to Mechanism in Organic Chemistry: Peter Sykes.
4. Synthetic Organic Chemistry: H. O. House
5. Principles of Organic Synthesis: R. O. C. Norman
6. Organic Chemistry: Clayden and Greeves
7. Mechanism and Structure in Organic Chemistry: E. S. Gould

CHEC-203 : Physical chemistry

04 Hrs/Week

Credits: 04

Marks: 100

Unit -I: Quantum Chemistry-I

12 hrs

The Schrodinger equation, particle in a one dimensional box, Eigen values and Eigen functions, operators, properties of quantum mechanical operators, Hermitian, Linear, Ladder, Hamiltonian and angular momentum operators.

Particle in three dimensional box, harmonic oscillator, rigid rotator and numericals.

Unit -II: Quantum Chemistry-II

12 hrs

Term symbols and selection rules, spin-orbital coupling, the variation theorem, non-degenerate perturbation theory and applications. Huckel molecular orbital theory of conjugated systems, application to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene and benzene, numericals.

Unit-III: Phase Rule

12 hrs.

Recapitulation of phase rule and terms involved in it, one component system, two component systems (solid-solid, solid-liquid and liquid-liquid), reduced phase rule, three component systems, partially miscible three liquid systems : one partially miscible pair, two partially miscible pairs, three partially miscible pairs, systems composed of two solids and a liquid : crystallization of pure components only, formation of binary compounds, formation of ternary compounds, formation of solid solutions, partial miscibility of solid phases, numericals.

Unit-IV: Crystallography

12 hrs

Classification of solids on the basis of shapes, and bonding, crystal lattice and unit cell, laws of crystallography crystal symmetry, symmetry elements, lattice planes and their designations, liquid crystals.

Principle of crystal structure. close packing of atoms, packing of equal sized spheres in HCP, CCP, BCC structures. packing in ionic solids, atomic packing factor in crystal structures, ionic radius, radius ratio rule, (3, 4, 6, 8 coordinate structures). octahedral and tetrahedral voids, isomorphism and polymorphism, numericals.

Unit-V: Photochemistry

12 hrs

Absorption of light and nature of absorption spectra, electronic transitions. photo-dissociation and pre-dissociation. photo-oxidation, photo-reduction and photo-dimerization. photo-physical phenomenon. Jablonski diagram. photo-physical pathways of molecular de-excitation, difference between delayed fluorescence and phosphorescence, Stern-Volmer

equation, deviations from Stern-Volmer equation, concentration dependence of quenching and excimer formation, quenching of fluorescence formation of excimer and exciplexes.

References Books:

1. Quantum Chemistry : Ira N. Levine
2. Quantum Chemistry : R.K. Prasad
3. Quantum Chemistry : B.K. Sen
4. Principles of Physical Chemistry : Puri, Sharma, Pathania
5. Advanced Physical Chemistry : Gurdeep - Raj, Plenum.
6. Physical Chemistry : Maron and Prutton
7. Introduction to Molecular Photo-chemistry : C.H.J. Wells
8. Fundamentals of Photo-chemistry : Rohatgi-Mukherjee.
9. Photo-chemistry : J.G. Calvert & J.N. Pitts.
10. Photo-luminescence of solutions : C.A. Parker.
11. Photo-chemistry : A. Singh and R. Singh
12. Atkins's Physical Chemistry : Peter Atkins
13. Solid State Chemistry : D.K. Chakraborti
14. Solid State Chemistry and its applications : A.R. West.
15. The Determination of Molecular Structure : P.J. Wheatley.
16. Solid State Chemistry : N.B. Hannay.
17. Principles of Solid State : H.V. Keer.
18. Physical Chemistry : G.K. Vemulapalli.

CHEF-204: Analytical chemistry

02 Hrs/Week

Credits: 02

Marks : 50

Unit-I: General introduction of spectral methods of analysis.

15 hrs

Characterization of electromagnetic radiations, Regions of the spectrum, Interaction of radiations with matter - absorption, emission, transmission, reflection, dispersion, polarization and representation of spectra, basic elements of practical spectroscopy, resolving power, signal to noise ratio. Uncertainty relation and natural line width, natural line broadening, intensity of spectral lines, energy levels, selection rules, components of spectrometer and their functions.

Microwave spectroscopy: Rotation of molecules, rotational spectra, diatomic molecules - rigid diatomic molecules, intensities of spectral lines, effect of isotopic substitution, non-rigid rotator, the spectrum of non-rigid rotator, polyatomic molecules, technique and instrumentation in outline, applications, numerical problems.

Unit-II: Vibrational spectroscopy

15 hrs

Review of linear harmonic oscillator, the vibrating diatomic molecule, the simple harmonic oscillator, the anharmonic oscillator, the diatomic vibrating rotator, the vibration-rotation spectrum of carbon monoxide, breakdown of the Born-Oppenheimer approximation, the vibration of polyatomic molecules, overtones and combination frequencies, the influence of rotation on the spectra of polyatomic molecules, the influence of nuclear spin, symmetric top molecules, analysis by Infra-red technique - Group frequencies, outline of technique and instrumentation. **Raman spectroscopy:** Classical and quantum of theory of Raman effect, pure rotational, vibrational and vibrational-rotational Raman spectra, rule of mutual exclusion, overtone and combination vibrations, Rotational fine structure, outline of technique and instrumentation, applications.

References Books:

1. The Determination of Molecular Structure : P. J. Wheatley
2. Physical Chemistry : G. M. Barrow
3. Instrumental Methods of Chem. Analy. Chatwal and Anand.
4. A Text book of Phy.Chem. : A.S. Negi& S. C. Anand
5. Instrumental Methods of Chemical Analysis - Willard, Merritt, Dean &Seale
6. Instrumental Methods of Chemical Analysis - Chatwal, Anand
7. Instrumental Methods of Chemical Analysis - B.K. Sharma
8. Instrumental Methods of Chemical Analysis -R.D. Braun
9. Analytical Chemistry : Skoog and West

10. Principles of Instrumental Analysis: Skoog and West.
11. Fundamentals of Molecular Spectroscopy: Banwell.
12. Atomic and Molecular Structure : ManasChanda
13. Molecular Spectroscopy : B.D. Acharya
14. Molecular Spectroscopy: Dyer.
15. Organic Spectroscopy: P.S. Kalsi (6th Edition).
16. Spectroscopic Methods in Organic Chemistry : D.H. Williams and I.Fleming.
17. Spectrometric Identification of Organic Compounds : R.M. Silverstein, Morrill and G.C. Bassler
18. Introduction to Spectroscopy : Pavia, Lampman and Kriz (3rd Edition)
19. Organic Spectroscopy: William Kemp (3rd Edition).
20. Quantum Chemistry- B. K. Sen
21. Inorganic Chemistry - Atkins and Shriver.

-

Unit-I: Elemental methods of analysis**15 hrs**

Flame emission spectroscopy: Principles, instrumentation, interferences, limitations, applications and numerical. **Atomic absorption spectroscopy:** Introduction, principles, instrumentation, sources of EMR-hollow cathode lamps, temperature gradient lamps, cells, flames, furnaces, detectors, interferences, background corrections and use of AAS for qualitative and quantitative analysis

Electron Spectroscopy Photoelectron spectroscopy: Basic principles, ESCA- Introduction - ESCA - ESCA satellite peaks, spectral splitting, ESCA chemical shifts, Principle, instrumentation, applications, Auger electron spectroscopy, Ultraviolet photoelectron spectroscopy.

Unit-II: Ultraviolet- Visible Spectroscopy:**15 hrs**

Various Electronic transitions, chromophores, Auxochromers, Bathochromic and Hypochromic Shifts, Effect of solvent on electronic transitions, Woodward-Fieser rules for dienes, enones and aromatic compounds, Applications of U.V.

Infrared Spectroscopy

Characteristic vibrational frequencies of alkenes, alkynes, aromatic compounds, Carbonyl compounds, hydroxyl compounds, amines and metal-ligand complexes. Factors affecting IR group frequencies, overtones, combination bands and Fermi resonance. Applications of IR.

References Books:

1. The Determination of Molecular Structure : P. J. Wheatley
2. Physical Chemistry : G. M. Barrow
3. Instrumental Methods of Chem. Analy. Chatwal and Anand.
4. A Text book of Phy.Chem. : A.S. Negi& S. C. Anand
5. Instrumental Methods of Chemical Analysis - Willard, Merritt, Dean &Seale
6. Instrumental Methods of Chemical Analysis - Chatwal, Anand
7. Instrumental Methods of Chemical Analysis - B.K. Sharma
8. Instrumental Methods of Chemical Analysis -R.D. Braun
9. Analytical Chemistry : Skoog and West
10. Principles of Instrumental Analysis: Skoog and West.
11. Fundamentals of Molecular Spectroscopy: Banwell.
12. Atomic and Molecular Structure : ManasChanda
13. Molecular Spectroscopy : B.D. Acharya
14. Molecular Spectroscopy: Dyer.

15. Organic Spectroscopy: P.S. Kalsi (6th Edition).
16. Spectroscopic Methods in Organic Chemistry : D.H. Williams and I.Fleming.
17. Spectrometric Identification of Organic Compounds : R.M. Silverstein, Morrill and G.C. Bassler
18. Introduction to Spectroscopy : Pavia, Lampman and Kriz (3rd Edition)
19. Organic Spectroscopy: William Kemp (3rd Edition).
20. Quantum Chemistry- B. K. Sen
21. Inorganic Chemistry - Atkins and Shriver.

CHEF- 206 : Review of literature

01 Hrs/Week

Credit: 01

Marks : 25

CHELI-207: Laboratory Course

06 Hrs/Week

Credits: 03

Marks: 50

List of experiments

I. Semi micro qualitative inorganic analysis

Identification of three acidic and three basic radicals including one rare earth from the given mixture [06 Mixture]

Note : Each mixture should contain different rare earth elements

II. Separation and estimation of amount of metal ions from the following mixture solutions

1. Copper- Barium
2. Iron –Aluminum
3. Copper- Iron

Reference Book

1. A Text book of Micro and Semi micro Qualitative Inorganic Analysis, IV edn, A. I. Vogel
2. A Text book of Quantitative Inorganic Analysis; A. I. Vogel
3. Practical Inorganic Chemistry- Pass Geoffrey and Haydn Sutcliffe.
4. Advanced Practical Inorganic Chemistry- Gurudeep Raj;.
5. Vogel's Qualitative Inorganic Analysis, VII Edn. Orient Longman Ltd. D. Svehla.

Scheme of Marking

I. Semi micro Inorganic analysis	25 Marks
i. Preliminary Test	03 Marks
ii. Acidic radicals along with C.T.	09 Marks
iii. Group identification of basic radicals	04 Marks
iv. Basic radicals along with spot test & C.T	09 Marks
II. Separation and Estimations of binary mixture of metal ions:	15 Marks
i. Observation Table :	05 Marks
ii. Calculation & Results :	10 Marks
III. Journal and Viva-Voce	10 Marks

--

CHELO-208: Laboratory course**06 Hrs/Week****Credits: 03****Marks: 50**

List of experiments**1. Qualitative Organic Analysis:****Marks: 25**

Separation, purification and identification of binary (**Solid-Liquid**) mixtures.

The separation should be carried out using Chemical method.

The two components are solid-liquid mixtures.

Student should submit the purified samples of the separated compounds and prepare a suitable derivative of the two compounds separated out.

Note : Analysis of at least five mixtures should be carried out.

2. Single Stage Preparations:**Marks: 15**

i) *p*-Bromo acetanilide from acetanilide.

ii) 1,4-dichlorobenzene from *p*-chloroaniline

iii) Benzophenone from benzene (Friedal Craft)

Note: i) The preparations should be carried out using (0.02 to 0.05 mole) of the starting material.

ii) The yield, melting point and TLC of the recrystallised product should be recorded.

Note : Student will not be allowed for practical examination if his/her record book is not completed and certified.

3. Record Book & Viva**Marks: 10****Scheme of Marking:****1. Qualitative Organic Analysis (Analysis of one Component is Compulsory)****Marks**

i) Type of the mixture

07

ii) Preliminary test

02

Analysis of the individual components:

iii). Detection of Elements

03

iv) Detection of functional groups

03

v) Determination of MP/BP

04

vi) Preparation of the derivative

04

vii) Identification (Spotting)

02

2. Preparation

i) Brief Experimental procedure along with mechanism and calculations

05

ii) Submission of recrystallized product

05

iii) Yield and MP of pure product

05

List of experiments**A. Instrumentation.**

1. Determination of dissociation constants of phosphoric acid potentiometrically.
2. Determination of dissociation constants of weak acid potentiometrically.
3. Determination of acidic and basic dissociation constants of an amino acid and its isoelectric point.
4. Determination of equilibrium quotient for the formation of monothiocynato iron (III) complex.
5. To study the kinetics of mutarotation of glucose/fructose polarographically.

B. Non-Instrumentation.

1. To study the adsorption of acetic acid from aqueous solution by activated charcoal and examine the validity of Freundlich and langmuir's isotherm.
2. To construct the phase diagram for three component system (chloroform-acetic acid-water).
3. To study auto catalysis reaction between potassium permanganate and oxalic acid.
4. Determine the rate constant of the reaction between potassium persulphate and potassium iodide having equal/unequal concentration of the reacting species.
5. To study the variation of viscosity with the composition of mixtures (ethanol-water-HNO₃-chloroform) and to determine the formation of complex between two liquids.

Note : Student will not be allowed for practical examination if his/her record book is not completed and certified.

Scheme of marking :1) Experiment I
(Instrumentation)

Marks

i) Observation :	10
ii) Calculation :	05
iii) Graph :	05
Accuracy & Results :	05
Record book & Viva :	05

Experiment -II
(Non-instrumentation)

Marks

08
04
04
04
05

Reference Book

1. Systematic experimental physical chemistry – T. K. Chondhekar & S.W. Rajbhoj
2. Experiments in chemistry – D.V. Jahagirdar