

**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 2<sup>nd</sup> year (3<sup>rd</sup> 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.

<b>Semester- I (Core and Foundation Courses)</b>				
<b>Paper No.</b>	<b>Course Title</b>	<b>Teaching (hrs/week)</b>	<b>Marks</b>	<b>Credits</b>
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
<b>Total Credits for Semester I: 25 (Theory: 16; Laboratory: 09)</b>				

<b>Semester- II (Core and Foundation Courses)</b>				
<b>Paper No.</b>	<b>Course Title</b>	<b>Teaching (hrs/week)</b>	<b>Marks</b>	<b>Credits</b>
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
<b>Total Credits for Semester II: 26 (Theory: 17; Laboratory: 09)</b>				

## CHEC-101: Inorganic Chemistry

04 Hrs/Week

Credits: 04

Marks : 100

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### 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 ( $\sigma_v$ ,  $\sigma_h$ ,  $\sigma_d$ ), 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 its 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

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## CHEC-102: Organic Chemistry

04 Hrs/Week

Credits: 04

Marks : 100

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### 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  $\pi$ -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  $SN^2$ ,  $SN^1$  mixed  $SN^1$  and  $SN^2$  and SET mechanisms. The neighbouring group mechanism, Neighbouring group participation by  $\pi$  and  $\sigma$ -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

## CHEC- 103 : Physical Chemistry

04 Hrs/Week

Credits: 04

Marks : 100

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### 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

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## CHEF-104 : Analytical Chemistry

02 Hrs/Week

Credits: 02

Marks : 50

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### 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 Ed<sup>n</sup>. 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.

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**COM - 100 : Constitution of India**

**02 Hrs/Week**

**Credits: 02**

**Marks : 50**

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**Unit I : History of Making of the Indian Constitution. [ 04 Hrs]**

1.1 History

1.2 Drafting Committee, ( Composition & Working)

**Unit II : Philosophy of the Indian Constitution [ 06 Hrs.]**

2.1 Preamble

2.2 Salient Features

**Unit III : Contours of Constitutional Rights & Duties [ 12 Hrs.]**

**3.1 Fundamental Rights**

\* Right to Equality, \* Right to Freedom, \* Right against Exploitation ,\* Right to Freedom of Religion , \* Cultural and Educational Rights, \* Right to Constitutional Remedies

3.2 Directive Principles of State Policy, 3.3 Fundamental Duties

**Unit IV : Organs of Governance [ 08 Hrs.]**

**4.1 Parliament**

\* Composition, \* Qualifications and Disqualifications, \* Powers and Functions

**4.2 Executive**

\* President, \* Governor, \* Council of Ministers,

**4.3 Judiciary**

\* Appointment and Transfer of Judges, \* Qualifications, \* Powers and Functions

**.. References :-**

1. *The Constitution of India*, 1950 (Bare Act),

Government Publication.

2. Dr. S. N. Busi, *Dr. B. R. Ambedkar framing of Indian Constitution*,

1st Edition, 2015.

3. M. P. Jain, *Indian Constitution Law, 7th Edn.*, Lexis Nexis, 2014.

4. D.D. Basu, *Introduction to the Constitution of India*, Lexis Nexis, 2015

5. M.P. Jain, *Outlines of Indian Legal and Constitutional History*, Lexis Nexis, 2014.

**Note : All latest volumes of above mentioned books must be preferred. The above list of books is not an exhaustive one**

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## CHELI -105 : Laboratory Course

06 Hrs/Week

Credits: 03

Marks : 50

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### List of experiments

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

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|---|---|--|
| 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

<b>Preparation &amp; estimation of percentage of metal ion Metal Complexes</b>	<b>25 Marks</b>
i). Yield of complexes	15 Marks
ii). Observation table, Calculation & Results	10 Marks
<b>II. Separation and Estimations of binary mixture of metal ions:</b>	<b>15 Marks</b>
i). Observation table	05 Marks
ii). Calculation & Results	10 Marks
<b>III. Journal and Viva-Voce</b>	<b>10 Marks</b>

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**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  $\text{BaSO}_4$ .
4. Determine the  $\text{pK}_1$  and  $\text{pK}_2$  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  $\text{CH}_2$ , 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)	Max. Marks	Experiment -II ( Non-instrumentation)	Max. Marks
i) Observation :	10		08
ii) Calculation :	05		04
iii) Graph :	05		04
Accuracy & Results :	05		04
Record book & Viva :	05		05

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

Terms, Inter-electronic repulsion, spin orbit coupling, ground terms, determination of term 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  $\beta$  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<sup>-</sup> group, Compounds containing NO<sup>+</sup> 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 ( $Re_2Cl_8$ )<sup>2-</sup>, Trinuclear ( $ReCl_3$ )<sub>3</sub>, Tetranuclear ( $W_4(OR)_6$ ) and Hexanuclear ( $Mo_6Cl_6$ )<sup>4+</sup> 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

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## CHEC- 202: Organic chemistry

04 Hrs/Week

Credits: 04

Marks: 100

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### 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  $S_N^{Ar}$ ,  $S_N^1$ , 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, pinacole-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

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### 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. Atkin'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. Hannary.
17. Principles of Solid State : H.V. Keer.
18. Physical Chemistry : G.K. Vemulapalli.

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## CHEF-204: Analytical chemistry

02 Hrs/Week

Credits: 02

Marks : 50

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### 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.

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**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.

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**CHEF- 206 : Review of literature**

**01 Hrs/Week**

**Credit: 01**

**Marks : 25**

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1. Fundamentals of literature survey
2. Information of search engines like Google, SCOPUS, etc
3. Compilation of literature
4. Brief literature review on the given topic
5. Preparation of review articles
6. Evaluation of review written by students

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**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**

<b>I. Semi micro Inorganic analysis</b>	<b>25 Marks</b>
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
<b>II. Separation and Estimations of binary mixture of metal ions:</b>	<b>15 Marks</b>
i. Observation Table :	05 Marks
ii. Calculation & Results :	10 Marks
<b>III. Journal and Viva-Voce</b>	<b>10 Marks</b>

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**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)**

	<b>Marks</b>
i) Type of the mixture	07
ii) Preliminary test	02
<b>Analysis of the individual components:</b>	
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
<b>2. Preparation</b>	
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-HNO<sub>3</sub>-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	Experiment -II ( Non-instrumentation)	Marks
i) Observation :	10		08
ii) Calculation :	05		04
iii) Graph :	05		04
Accuracy & Results :	05		04
Record book & Viva :	05		05

**Reference Book**

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

**DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY,  
AURANGABAD.**

**DEPARTMENT OF CHEMISTRY**



# **SYLLABUS**

**M. Sc. Inorganic Chemistry**  
(Semester III & IV)

**Choice Based Credit and Grading System**

**Effective from : June 2017**

The following will be the Choice Based Credit and Grading System structure of revised syllabus for M. Sc. III & IV semester Inorganic Chemistry effective from June 2017.

Semester	Paper Nos.	Title of Paper	Teaching (hr)/week	Marks	Credits
III- Semester	CHEEC-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 <b>OR</b>	04	100	04
	CHEEI -305	Environmental chemistry <b>OR</b>	04	100	04
	CHEEI- 306	Solid state chemistry	04	100	04
	CHELI- 307	Laboratory course	06	50	03
	CHELI- 308	Laboratory course	06	50	03
	CHELI- 309	Laboratory course	06	50	03
IV semester	CHECI -401	Nuclear chemistry	02	50	02
	CHECI -402	Photoinorganic chemistry	04	100	04
	CHECI -403	Therapeutic bioinorganic and chemistry of forensic materials	04	100	04
	CHEEI -404	Organo transition Metal Chemistry, <b>OR</b>	04	100	04
	CHEEI -405	Polymer chemistry , <b>OR</b>	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

## CHESC-301: Structural elucidation by spectral method

04 Hrs/Week

Credits: 04

Marks 100

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### UNIT-I: Nuclear Magnetic Resonance Spectroscopy ( $^1\text{H}$ NMR) [12hrs]

Elementary ideas (Recapitulation); Spin-spin couplings, Different types of couplings, factors affecting on coupling constants, Karplus equation, Spin systems (AB, AX, ABX, AMX), Rate processes, spin decoupling, shift reagents, Nuclear Overhauser effect (NOE), INEPT and INADEQUATE.

### UNIT-II: $^{13}\text{C}$ Nuclear Magnetic Resonance Spectroscopy [12hrs]

Elementary ideas, instrumental problems, chemical shifts (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbons); Effect of substituents on chemical shifts.

### UNIT-III: Mass Spectroscopy [12hrs]

Introduction, ion production (EI, CI, FD and FAB), ion analysis, ion abundance, factors affecting on fragmentation, fragmentation of different functional groups, molecular ion peak, isotopic peaks, metastable peak, Nitrogen rule, McLafferty rearrangement, Retro-Diels-Alder reaction.

### UNIT-IV [12hrs]

Problems based on joint applications of UV, IR,  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and Mass spectroscopy.

### UNIT-V [12hrs]

**Mossbauer spectroscopy:** Principle, factors affecting the line position and shape, isomer effect and Quadrupole splitting iron salt like compounds, complexes, carbonyl compounds (temperature dependence of isomer shift and Quadrupole splitting in simple compound and coordination, polynuclear complexes), Numericals. **Electron Spin Resonance Spectroscopy:** Introduction, principle of ESR spectroscopy, presentation of spectrum, hyperfine splitting in various structures, hyperfine splitting diagram of representative examples, factors affecting the magnitude of 'g' values, Zero field splitting, Kramer's degeneracy, Anisotropy in the hyperfine coupling constant, electron delocalization, instrumentation and applications.

### Reference Books:

1. Introduction to Spectroscopy: D. L. Pavia, G. M. Lampman, G. S. Kriz
2. Spectrometric Identification of Organic Compounds: R. M. Silverstein & F. X. Webster
3.  $^{13}\text{C}$  NMR Spectroscopy: G. C. Levy, R. L. Lichter, G. L. Nelson
4. Spectroscopic Methods in Organic Chemistry: D. H. Williams & I. Fleming Absorption

5. Spectroscopy of Organic Compounds: V. M. Parikh
6. Mass Spectrometry: K. G. Das & James
7. Coordination Chemistry by Experimental Methods: K. Barger
8. Coordination Chemistry vol. I: E. Martell
9. Physical Methods for Chemistry: R. S. Drago
10. Structural Methods in Inorganic Chemistry: E. A. V. Ebsworth & D. W. H. Rankin
11. Organic Structure Analysis: Philips Crews

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## CHECI- 302: Bioinorganic and supramolecular chemistry

04 Hrs/Week

Credits : 04

Marks : 100

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### Unit- I: Metalloenzymes:

[12 hrs]

Structural and functional relationships and mechanisms of enzymatic reaction in the following metalloenzymes. **Zinc Enzymes:** carbonic anhydrase and carboxypeptidases, **Copper Enzymes:** super oxide dismutases **Iron Enzymes:** catalase and peroxidases, **Molybdenum Enzymes:** nitrogenase and xanthine oxidase, Coenzyme Vitamin: B-12

### Unit-II: Metal Nucleic Acid Interactions:

[12 hrs.]

Introduction, nucleic acid structures, structures and binding sites in nitrogen bases, phosphates and sugar base. Coordination complexes of nucleic acids and their bases with metal ions. Hydrogen bonding, redox reaction and hydrolytic reaction of nucleic acids mechanisms of these reactions, nature's role, pharmaceutical role, catalytic role

### Unit-III: Supramolecular chemistry

[12 hrs]

Basic concepts and principles of supramolecular chemistry, Host-Guest interactions, Molecular Recognition, spherical recognition, anionic receptors, porphyrin-sapphyrin systems, organometallic receptors, tetrahedral multiple and neutral molecular cleft recognition, enzyme models, molecular receptors, design and synthesis.

### Unit-IV: Supramolecular reactions and catalysis

[12hrs]

- Catalysis by anion, cation and metal receptor molecules and co catalysis.
- Molecular and supramolecular devices : likes Photonic, Electronic and ionic devices..

### Unit-V: Storage of metals and transport across the membrane

[12hrs]

The fluid mosaic model of membrane, types of transport and their mechanism, Transport and storage of alkali and alkaline earth metals, Na<sup>+</sup>-K<sup>+</sup> pump, calcium pump. Gibbs-Donnan equilibrium, Iron transport proteins and compounds.

### Reference Books:

- Bioinorganic chemistry -Bertini Ivano, Gray H. B., Lippard S. J. & Valentine J. S.
- Principles of Bioinorganic chemistry - S. J Lippard & M. J. Berg
- Inorganic Biochemistry, ( Vol.I & II) - G. L. Eicchorn.
- Bioinorganic chemistry :- A. K. Das.



5. Bioinorganic chemistry - R. W. Hay.
6. Bioinorganic chemistry - Chatwal G. R. & A. K. Bhagi.
7. Supramolecular chemistry -Lehn J. M.
8. Bioinorganic & Supramolecular chemistry - Chatwal G. R. & A. K. Bhagi.
9. Bioinorganic, Bioorganic & Supramolecular chemistry Kalasi P. S.
10. Supramolecular organometallic chemistry J. L. Atwood and Jonathava W. steed, Macel  
Jekkar Publisher
11. Supramolecular Organometallic chemistry -Jean Marie-Lehn.
12. Elements of bioinorganic chemistry - G N Mukharji & Arvind Das

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## CHECI- 303: Applied inorganic chemistry

04 Hrs/Week

Credits: 04

Marks : 100

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### Unit –I: Basic concept of zeolites

[12 hrs]

Introduction, definition, classifications on the basis of morphological appearance, SBU, substitution of other iso-electronic metal ions, types of pore size. Lowenstein's rule. pore and channels, channel dimensions, shape of the pore opening, nomenclature of zeolites, structural aspect of zeolites, acidity of zeolite, identification of acidic sites, nature of active sites, synergetic effects, shape selectivity.

### Unit-II: Synthesis of zeolites

[12 hrs]

General methods for synthesis of zeolite, hydrothermal treatment, mechanism of aluminosilicate formation during Sol-Gel, co-precipitation process, factors affecting the zeolite formation. Modification of zeolites, Oswald's rules of successive transformation, crystallization and its identification, factors affecting crystallization, template theory, organic additives, crystallizing zeolites, ZSM-5 from an organic free solvent system, synthesis in nonaqueous solvents.

### Unit-III: Characterization and applications of zeolite

[12 hrs]

General characterization techniques for analysis of zeolites, Details on FTIR, Pyridine adsorbed- IR analysis, XRD analysis,  $^{27}\text{Al}$  MAS NMR and  $^{29}\text{Si}$  MAS NMR analysis, Temperature programmed desorption (TPD), probe molecules for TPD analysis,  $\text{NH}_3$ - TPD and  $\text{CO}_2$ - TPD. Applications of zeolite, Zeolite catalyzed reactions, water softening.

### Unit-IV: Fundamentals of catalysis

[12 hrs]

Catalysis, types of catalysis, catalyst, properties of catalyst, classification of catalysts, Sabtier's principle, classification of solid catalysis, fundamentals of heterogeneous catalysis, factor affecting the catalyst performance, promoters, types of promoters, Inhibitors, catalyst poisoning, overview on heterogeneously catalyzed process in industry.

### Unit-V: Basic Chemical Calculations:

[12 hrs.]

Moles, Mole fraction, percent composition, weight & volume percent analysis of solid in composition, Material balance involving chemical reaction: Introduction, material balances, Concept of Selectivity, Conversion, and numericals. Principle of green chemistry, Atom economy numericals

**Reference Books:**

1. Molecular sieves: Principles of synthesis and Identifications R-Szostak.
2. Atlas of zeolite framework type; Ch. Barlocher, W M. Meier , D. H. Olson; 5<sup>th</sup> rev.  
Ed. Elsevier Amsterdam 2001
3. Molecular Sieves Science and Technology vol I & II, H G Karge , J Weitkamp- Springer
4. Molecular Sieves Science and technology ; H. G. Karge, J Weitkamp Vol I to V , Springer
5. Industrial catalyst- A Practical Approach , Jens Hygen, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany
6. Stoichiometry (SI Units): B.I. Bhatt & S.M. Vora.
7. Heterogeneous Catalysis and Solid Catalysts , Olaf Deutschmann, Helmut Knozinger, Karl Kochloefl, Thomas Turek, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim
8. Green chemistry and catalysis – Roger A . Sheldon , Isabel Arends , Ulf Hanefeld . Wiley VCH

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## CHEEI- 304: Chemistry of materials

04 Hrs/Week

Credits: 04

Marks : 100

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### **Unit-I: General introduction & synthesis of nanomaterials by physical methods [12 hrs]**

Objective of study, synthesis of nanoparticles by physical method, mechanical methods- high energy ball milling, melt mixing, method based on evaporation, physical vapour deposition with consolidation. Ionized cluster beam deposition. Laser vaporization, Laser pyrolysis, sputter deposition, electric arc deposition, Chemical Vapour Deposition (CVD).

### **Unit-II: Synthesis of Nanomaterials by Chemical Methods [12hrs]**

Introduction, colloids and colloids in solution, interaction of colloids and medium, colloids in vacuum, colloids in medium, effect of charge on colloids, steric repulsion, synthesis of colloids, growth of nanoparticles, synthesis of metal and semiconductor nanoparticles by colloidal route, Langmuir-Blodgett (L-B) method, sol gel method, electrochemical method.

### **Unit-III: Analysis Technique [12hrs]**

Introduction, microscopes, electron microscopes, SEM, TEM, Scanning probe microscope (SPM), Scanning Tunneling microscope, Atomic force microscope, X-ray diffraction, UV-visible and IR spectroscopy.

### **Unit-IV: Properties, types and application of Nanomaterials [12hrs]**

- i). Properties of nanomaterials – Mechanical, electrical, optical, magnetic, semiconductor.
- ii). Some special nanomaterials – Carbon nanotubes, porous silicon, Arogels, Zeolites.
- iii). Application – Electronic, energy automobiles, sport and toys, textile, cosmetics, domestic appliances, biotechnology, medical, space, defence & environment.

### **Unit-V: Imperfections in solids [12hrs]**

Perfect and imperfect crystal, point defects, stoichiometric defects, Schottky & Frankle defects, thermodynamics of their formation, colour centers, Non-stoichiometric defects, metal excess and metal deficiency defects, line imperfections, Edge dislocation, Screw dislocation, Burgers circuits, Surface imperfections, grain boundaries & stacking faults.

Theories of solid states – free electron theory, band theory, refinement to simple band theory.

### **Reference Books:**

1. Solid State Chemistry and applications- A.R. West (John Wiley and Sons)
2. Principles of the Solid State- H.V. Keer (Wiley Eastern Limited)

3. Nanotechnology: Principles and practices- Sulabha K. Kulkarni (capital Pub. Co.)
4. NANO- The next revolution –Mohan Surendra Rajan(National book Trust, India)
5. The British Glass Website- Types of Glass://www.britiglass.org.uk.
6. Fundamental of Nanotechnology – Gabor L. Hornyak, John J. Moore, Harry F. Tibbals, Joydeep Dutta.
7. Recent advances in the liquid phase synthesis of Inorganic Nanoparticles- B. L. Cushing
8. V. L. Kolesmichenko & C.J.O”.Connor Chemical Review 104, 3893-3946.(2004)

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## CHEEI-305: Environmental chemistry

04 Hrs/Week

Credits : 04

Marks : 100

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### Unit-I: Air Pollution

[12 hrs]

General considerations: polluted air, Types of pollution and units of measurements. Air quality standards, Sampling, Monitoring, Analysis of CO, Sources and sinks of CO pollution, Effects of CO on plants and humans, Control of CO pollution, Analysis of oxides of nitrogen, NO<sub>x</sub> sources and sinks of NO<sub>x</sub> pollution, Control of NO<sub>x</sub> pollution, Hydrocarbons and photochemical smog and its control, Analysis of hydrocarbon in exhaust gasses, Petrol and air, Sulphur dioxide sources, Analysis and control, Acid rain particulates and their effects on human and climate, Control of particulates.

### Unit-II:

[12 hrs]

**Water Pollution:** Aquatic environment, Water pollutants, Sampling of water and its preservation Trace metals in water, Chemical speciation with special reference to Copper, Lead, Mercury and Arsenic. Water quality standards Water quality parameters.

**Oxygen Demanding Wastes:** Dissolved oxygen, Biological oxygen demand, Monitoring techniques and methodology with special reference to ammonia, Nitrates, Nitrites, Fluorides, Cyanides, Total hardness, Lead, Cadmium and Mercury. Detection and control of Detergents, oils, Pesticides, Sewage treatment.

### Unit-III:

[12 hrs]

**Chemical toxicology :**Toxic chemicals in environment, Impact of toxic chemicals on enzymes, Biochemical effects of Arsenic, Cadmium, Lead, Mercury, Carbon monoxide, Sulphur dioxide, Pesticides and Carcinogens.

**Soil analysis:** Sampling of soil, Determination of water holding capacity, Determination of total nitrogen, phosphorous and sulphur in soil.

### Unit-IV:

[12 hrs]

**Industrial pollution:** Pollution due to cement industry, Distillery, Pharmaceutical (Drug) industries, Sugar industry, Paper and pulp industries, Thermal power plants, Nuclear power plants, Metallurgical industries, Polymer industries. Recycle, reuse, recovery, disposal, and management of solid industrial waste.

## Unit-V: Pesticides and Environmental pollution

[12 hrs]

Types of pesticides, , Insecticides and Herbicides . Effect of pesticides, Insecticides and Herbicides on environment , Physicochemical decomposition of pesticides, , Insecticides and Herbicides by soil microorganism and other living organism .

### Reference Books:

1. A. K. De, Environmental Chemistry, Wiley Eastern Ltd. New Delhi.
2. S. L. Chopra and J. S. Kanwar, Analytical, Agricultural Chemistry, Kalyani Publishers, New Delhi.
3. Environmental chemistry , V P Kudesia , Pragati prakashan , Meerut.
4. R. K. Trivedy and P. K. God, Chemical and biological methods for water pollution studies, Environmental publications, co. New Delhi.
5. L. A. Richards, Diagnosis and improvement of saline and alkali soils. Oxford IBH publications co. New Delhi.
6. S. M. Khopkar, Environmental chemistry, Environmental pollution analysis.
7. M. S. Creos and Morr, Environmental chemical analysis, American publications.
8. M. Sittig, Resources, Recovery and Recycling, Handbook of industrial waste.
9. Standard methods of water and waste water analysis, American public health association Washington D. C.
10. R. Gopalan and Amrutha Anand, "Environmental chemistry laboratory manual Emerald Publication.
11. Standards for water for drinking and other purposes, Bureau of Indian Standards India.
12. Guideline for drinking water quality recommendations of world health organization, Geneva.
13. B. K. Sharma and H. Kaur, Environmental Chemistry, Guel publishing house Meerut.
14. Thomas G. Spiro and William M. Stigliani, Chemistry of environment.
15. Green Chemistry: An Introductory Text, Mike Lancaster, Royal Society of Chemistry, (2002)
16. New Trends in green Chemistry, V.K. Ahluwalia and M. Kidwai, Anamaya Publishers New Delhi, (2004)

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## CHEEI-306 : Solid state chemistry

04 Hrs/Week

Credits : 04

Marks : 100

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### Unit-I: Solid state Reactions

[12 hrs]

General Introduction and principles, classification, Wagner reaction mechanism, Experimental procedures, Co-precipitations as precursor to solid state reaction, Kinetics of solid state reactions, Vapour Phase transport methods, Modification of existing structure by ion exchange and intercalation reactions,- Graphite intercalation compound, transition metal dichalcogenide and other intercalation compounds , Preparation of thin films, methods of characterization of thin films.

### Unit-I: Imperfections in solids

[12 hrs]

Perfect and imperfect crystals, point defects, stoichiometric defects, Schottky and Frenkel defects. Thermodynamics of their formation, color centers. Nonstoichiometric defects, metal excess and metal deficiency defects. Line imperfections, edge dislocation and screw dislocations, Burgers circuits. Surface imperfections, grain boundaries and stacking faults.

### Unit-III: Theories of solid state and electronic properties

[12 hrs]

Free electron theory, Conduction by free electrons, Band theory, refinement to simple band theory, band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors, semiconductor material and their fabrication. **Super conductivity:** conventional super conductors, organic super conductors(organic metals), fullerene, high temperature super conductors, organic charge transfer complexes, Applications

### Unit-IV Properties of solid

[12 hrs]

**Optical properties:** Luminescence and phosphors, lasers, photoconduction, photoelectric effects. **Magnetic Properties:** Behavior of substances in a magnetic field, classification of magnetic materials, effect of temperature, magnetic domains and hysteresis. **Electrical properties:** Thermoelectric effects, Thomson effects, Peltier effect, seebeck effect, thermocouples, Hall Effect, Dielectric materials, Ferro, Pyro, Piezo electricity and their relations. Applications.



## Unit-V Glass and Ceramics

[12 hrs]

**Glass:** Introduction, physical and chemical properties of glass. Methods of manufacture of glass, thermodynamics of glass formation, kinetics of crystallization and glass formation, types of glasses, sodalime glass, lead or flint glass, borosilicate glass, glass fiber, aluminosilicate glass, alkali-barium silicate glass, colored glass, opal glass, safety glass, technical glass, glass ceramics, optical (crookes) glass, sealing glass.

**Ceramics:** Introduction, classification, porous and non-porous materials wastes, clay and its properties, primary and secondary clays. Manufacturing process, glass ceramics.

### Reference Books:

1. Solid state chemistry and its applications – A. R. West (John Wiley and sons)
2. Principles of the solid state – H. V. Keer (Wiley Eastern Limited)
3. Material science and engineering – V. Raghavan (prentice hall of India)
4. Principles of electronics – V. K. Mehta (S. Chand and Co.)
5. Engineering Chemistry - P. C. Jain and M. Jain (Shanpat Rai and Sons)
6. Industrial chemistry – B. K. Sharma (Goel Publishing House)
7. The British Glass Website- Types of Glass: <http://www.britglass.org.uk>.

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**I. Prepare and estimate the percentage of metal ion in the metal complex and their spectral studies**

1. Tris (thiourea) Copper(II) Sulphate
2. Bis (thiourea) Zinc (II) sulphate
3.  $\text{NH}_4[(\text{Cr}(\text{III})(\text{C}_2\text{O}_4)_3]$
4.  $[\text{Ni}(\text{II}) (\text{Salicyldoxime})_2 ]$
5.  $[\text{Copper (II) (Acetyl acetone)}_2]$
6. Manganese (II) Phthalocyanine
7.  $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4 \cdot \text{H}_2\text{O}$
8.  $[\text{Co}(\text{NH}_3)_4\text{CO}_3]\text{NO}_3$
9.  $\text{K}_3[\text{Cr}(\text{CNS})_6] 4\text{H}_2\text{O}$
10.  $\text{K}_3[\text{Cr}(\text{C}_2\text{O}_4)_3]$
11.  $[\text{Cr}(\text{urea})_6]\text{Cl}_2 \cdot 3\text{H}_2\text{O}$

**II . Estimation**

1. Separation and estimation of Zn(II) and Cd(II) from given mixture using Amberlite IRA 400 anion exchange resin
2. Separation and estimation of Zn(II) and Mg(II) from given mixture using Amberlite IRA 400 anion exchange resin
3. Determine the Total hardness of water by using EDTA
4. Determine the percentage of chlorine from bleaching powder using Volhard method
5. Determination of iron content from given sample by using 8- hydroxyquinoline as extractant

**Reference Books:**

1. A Text book of Quantitative Inorganic Analysis; A. I. Vogel
2. Practical inorganic chemistry; Pass Geoffrey and haydn Sutcliffe.
3. Advance Inorganic Analysis – S K Agarwala, Keemti Lal , Pragati Prakashan
4. Advanced Practical inorganic chemistry; Gurudeep Raj.
5. Experiments in Chemistry, D. V. Jahagirdar, Himalaya Publishing House

**Scheme of marking**

I. Preparation of complexes	25 Marks
II. Estimation	15 Marks
III. Journal and viva voce	10 Marks

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## CHELI-308 : Laboratory course

06 Hrs / Week

Credits : 03

50 Marks

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### I Spectrophotometer:

1. Estimate the amount of copper and bismuth ions using EDTA photometric titration method
2. Determine the stability constant, empirical formula,  $\lambda_{\max}$ . by job's method, mole ratio and slope ratio method.
3. Determine the  $pK_a$  of Methyl red indicator

### II. $P^H$ metrically

1. Determine the  $P_k$  value of benzoic acid by using irrivaing Rossotgi method. by  $P^H$  metric method and metal ligand stability constant of its complex.
2. Determine the  $P_k$  value of Glycine by using irrivaing Rossotgi method. by  $P^H$  metric
3. Determine the metal ligand stability constant of copper benzoate complex by  $pH$  metric method.

### III. Conductometry

1. Analyze the acid mixture hydrochloric acid and acetic acid by conductometric method.
2. Analyze the mixture of copper sulphate, hydrochloric acid and acetic acid by conductometric method.
3. Determine the stability constant and composition/formula of lead oxalate by conductometric method.

### IV. Potentionmetry

1. Determine the redox potential of Fe(II)/Fe(III) system and hence determine the number of electron involved in the system using  $K_2Cr_2O_7$  by potentiometric method.
2. Determine the amount of chloride, bromide and iodide in the given sample by potentiometric method.

### V. Turbidometry

1. Determine the sulphate content of the given sample using turbidometric titration.

### VI. Flame photometry:

1. Estimate the amount of sodium/potassium from the given sample

### Reference Books

1. Systematic experimental physical chemistry – T. K. Chondhekar & S.W. Rajbhoj
2. Experiments in chemistry – D.V. Jahagirdar
3. Textbook of quantitative Inorganic Analysis – IV Edn. J. Bassett, R. C. Denny, G.H.Gefery and J. Mendham

### Scheme of marking

- |                              |          |
|------------------------------|----------|
| 1. Experiment - I            | 25 Marks |
| 2. Experiment- II            | 15 Marks |
| 3. Record book and Viva Voce | 10 Marks |

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**CHELI-309 : Laboratory course**

**06 Hrs / Week**

**Credits : 03**

**50 Marks**

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**I. Magneto chemistry : at least 05 sample**

1. Determine the number of unpaired electron in the given sample by Gouy's balance method

**Select the sample :** Copper sulphate, sodium sulphate, calcium carbonate, potassium ferrocyanide, potassium ferricyanide, coordination complexes

**II. Alloy analysis :**

1. Solder alloy analysis
2. Brass alloy analysis
3. Bronze alloy analysis.
4. Copper nickel alloy

**III. Ore analysis : Any 03**

1. Analysis of dolomite ore
2. Analysis of calcite ore
3. Analysis of Haematite ore
4. Analysis of bauxite ore.

**Scheme of marking**

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1. Analysis of ore/Alloy	25 Marks
2. Magneto chemistry	15 Marks
3. Journal and Viva Voce	10 marks

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## CHECI-401: Nuclear chemistry

02 Hrs/Week

Credits : 02

Marks: 50

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### Unit-I: Nuclear particles and its properties

[06 hrs ]

The fundamental particles, roll call of elementary particles, composition of the nucleus, theories of nuclear composition, nuclear properties, mass defect and binding energy, nuclear stability explained by different factors. Nuclear size and density,

### Unit-II: Nuclear models

[12 hrs]

The shell model and its salient features, periodicity in nuclear properties- magic numbers, forces of nuclear potential, energy level in nuclear potential well, the sequence of filling the orbital including models, nuclear configuration. The liquid drop model, and its details and The Fermi gas model.

### Unit-III Nuclear Reactions.

[12 hrs]

Definition and Bethes notation, nuclear reaction energetic, nuclear reaction and threshold energy, characteristics of nuclear reactions, types of nuclear reactions, conservation in nuclear reactions, nuclear reactions cross section, cross section and reaction rate, the compound nucleus theory, general properties of compound nucleus, optical model, direct interaction model, specific nuclear reactions- photonuclear reactions, stripping and pickup reactions evaporation, spallation, fragmentation, direct nuclear reactions, thermonuclear reactions.

### Reference Books.

1. Source of Atomic energy by s. Glasstance, D. Van Nostrand co. INC
2. Essentials of nuclear chemistry by H.J. Arnikaar 4<sup>th</sup> Edn, New Age International(p) Ltd.
3. Introduction to Nuclear By chemistry B. G. Harvey,
4. Nuclear chemistry by M. G. Arora & M. Singh Anmol publication, New Delhi
5. Elements of nuclear chemistry by A. K. Srivastav, P. C. Jain, S. Chand & Co.
6. A text book of Nuclear chemistry by C.V. Shekar Deminant publication & distribution, New Delhi.
7. Radiochemistry & nuclear chemistry, 3<sup>rd</sup> edn G. chappin, Butterwerth-Heinemann.

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## CHECI: 402 Photoinorganic chemistry

04 Hrs/Week

Credits: 04

Marks : 100

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### Unit-I: Basic concept of Photo Chemistry

[12 hrs]

Introduction to photochemistry, laws of photochemistry, Quantum yield, deviation in quantum yield, Experimental determination of quantum yield, Quantum yield and reactivity, life time of electronically excited state, kinetic aspects of photochemical reactions, temperature dependence of photochemical reaction, Methods used to study the kinetics of photochemical reaction: Flow methods, flash photolysis methods, numerical on quantum yield calculations.

### Unit-II: Physical properties of electronically excited molecules

[12 hrs]

Nature of changes on electronic excitation, potential energy diagram, shapes of absorption bands and Franck-Condon principle, emission spectra, environmental effect on absorption and emission spectra. **Photo physical process in electronically excited molecule:** Types of physical pathways, Jablonski diagram, theory of radiationless transition, theory of radiative process, bimolecular quenching, experimental results.

### Unit-III: Excited States of Metal Complexes

[12 hrs.]

Spectroscopic states of  $d^1$  to  $d^{10}$  configurations, Ligand field excited states of Co(II), Cr(III), Ru(II), Ru(III), Fe(II) and Rh(III) in an octahedral complexes. Excited states of organic ligand selection rules for electronic transitions. **Charge transfer photochemistry** :Introduction, charge transfer absorption spectra, types of charge transfer excitations and their energy level. Types of reactions observed by CTTM, Models of photoredox system.

### Unit-IV: Ligand field photo chemistry of transition metal complexes

[12 hrs]

Photochemistry Cr(III) of complexes : properties of ligand field excited states, Photo-substitutions reaction, Photo aquation reactions, photolysis rule, photoisomerization, photo-recimization, photoanation reactions, photo reactive excited state, doublet hypothesis, role of quartet excited states. Sensitizer, mechanism of photo sensitization, photosensitized aquation reaction. Photochemistry of Co(III) complexes : Energy level diagram, Photoaquations in Co(III) amine, Co(III) cyanide complexes. Photochemistry of Fe(II) low spin complexes, Ru(II) amine derivative complexes, Photo redox properties of (Ru(III) complexes.

### Unit-V: Photochemical reactions on solid surface:

[12 hrs]

Photo catalysis, photoreactive oxide materials, relation between band gap & energy, wavelength,

photo electron transfer mechanism, energy level diagram of solid acceptor and donor levels. Supported photo catalyst: Types of support & need . Semiconductor supported metal oxides for Photolysis of water. Decomposition of organic pollutants, experimental setup and photo degradation end product of organic moieties.

**Reference Books :**

1. Concepts of Inorganic Photo chemistry, W. Adamson
2. Photochemistry of Coordination Compound – V. Balzani and Carassiti , Academic press London & New York
3. Inorganic spectroscopy , A. B. P. Lever
4. Inorganic Chemistry, J. E. Huhey
5. Fundamental of Photochemistry, Rohatgi Mukherjee
6. Charge Transfer Excitation of Coordination compounds. Generation of reactive intermediate – A Vogler and H Kunkely
7. Metal complex Sensitizers in dye sensitized solar cells, Coord. Chem . Review , Andre Sarto Polo et al , 238, 1343-1361, **2004**
8. Metal centered ligand field excited state : Their roles in the design and performance of transition metal based photochemical moleculesar device , Paul S Wagenkecht and Peter C Ford , Coord. Chem. Review, 255, 591, **2011**.
9. D. Chatterjee , Visible light induced photo degradation of organic pollutants on dye Adsorbed TiO<sub>2</sub> surface : Bull. Cat. Soc. of. India 2,,56-58, **2004**

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## CHECI- 403: Therapeutic bioinorganic and chemistry of forensic materials

04 Hrs/Week

Credits : 04

Marks : 100

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### **Unit-I: Metal ions in carcinogenesis**

**[12 hrs]**

General and biochemical aspects of cancer, carcinogens and anticancer agents. Carcinogenesis and its mechanism. Role of metal complexes and Pt(II) and (IV) as anticancer agents, anticancer activity of rhodium, gold, copper, and cobalt complexes. Selenium and its biochemical role and its mechanism of cacinostatic actions. Some representative metallodrugs containing arsenic, antimony, gold, mercury and tin metal. Antibacterial, antifungal and antiviral activity of metal; complexes.

### **Unit- II: Chemistry of Forensic Materials**

**[12 hrs]**

Forensic toxicology, legal definition of poison and toxinology, human and cattlepoison, and its antidotes. Principle underlying removal of poison from the body and use of antidotes, corrosivepoison and its classification. Common household poisons. Characteristic sign, symptoms, treatment and medicolegal aspects of common household poisons, classifications of poisons according to their mode of action.

### **Unit- III: Concepts on metal ion toxicity**

**[12 hrs]**

Metal ion toxicity in man and animals. Introduction, general aspects of Pb(II), Cd(II), and Hg(II), biochemical and physiological effects caused due to Pb(II), Cd(II), and Hg(II) ion toxicity. Detoxifications of this metals using chelating agents.

### **Unit-IV: Interactions of metal ions and metal complexes**

**[12 hrs]**

Structure and functions of amino acids, proteins, peptides, enzymes nucleoside, nucleotide and comparative study of structures and functions of these biomolecules. Metal ion binding sites present in amino acids, peptides, proteins,enzymes, nucleoside and nucleotide. Interactions of metal ion and metal complexes with these biomolecules.

### **Unit-V: Metals in medicine**

**[12 hrs]**

Chelation therapy, Limitation of chelation therapy in metal ion detoxification , Zinc salt in the treatment of sickle cell anemia. Lithium therapy in psychiatric mind disorder, Metals used in diagonosis, radiodiagnostic agent, MRI and X-ray contrast agent , Bismuth and Vanadium compound in medicines, chelation and role of metal complexes in conventional drug resistant malaria

## Reference Books

Inorganic biochemistry – Guther L. Eicchorvol 1 and 2 volume (Elsevier Scientific Publishing Company Amsterdam 1973, London New York.

1. Pharmacological basis of therapeutic, 5<sup>th</sup> and 6<sup>th</sup> edition by –Louis S. Goodman, (Macmillan Publishing companyNC, New York, Toronto and London)
2. Metal ions in biological system - Helmut Sigel. Vol. 19 21, 22 - (Marcel Dekker INC, New York and Basel)
3. Metal ions in biological system (Concepts on metal ion toxicity) by Helmut Sigel. Vol.7- (Marcel Dekker INC, New York and Basel)
4. Modi's Medical Jurisprudence and Toxicology 22<sup>nd</sup> Edition.
5. Parikh's Textbook of Medical Jurisprudence, Forensic Medicine and Toxicology (Six Edition) By C. K. Prikh. (CBS Publishers & distributors 4596/1A 11, Daryagaing New Delhi- 11002
6. Bioinstrumentations – L Veerakumari , MJP publisher Chennai
7. Principles of bioinorganic chemistry – S. J Lippard & J M Berg , Mill Valley California
8. Elements of Bioinorganic - G N Mukherji, and Arbinda Das U N Dhur and Sons Pvt. Ltd Kolkatta

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## CHEEI- 404: Organo transition metal chemistry

04 Hrs/Week

Credits : 04

Marks : 100

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### Unit- I: General Properties of Organotransition Metal Compounds [ 12 hrs]

Definition, Classification based on the number of coordinated carbon (Hapticity), number of electrons donated by ligands, and type of bonding. Nomenclature, 16, 17, 18 Electron complexes and ligand substitutions, electron counting for common ligands and geometry of organo transition metal compounds.

### Unit-II: Alkyl, aryl Carbene and carbene transition metal compounds. [ 12 hrs]

General method of synthesis of alkyl and aryl transition metal compounds, (i.e Ti, V, W, Mn, Ir, Co, Fe ), Chemical properties, stability and decomposition pathways.

**Carbene transition compounds:** Types of carbene compounds, properties of carbene ligands, Synthesis of Fischer type carbene compounds, Chemical reaction on coordinated carbene compounds .**Carbyne transition metal compounds :** Synthesis and chemical properties

### Unit- III: Transition metal compounds with Unsaturated organic molecules: [12 hrs.]

**$\eta^2$  alkene transition metal compounds :** General methods of the synthesis, Chemical properties: Reaction with nucleophiles and Electrophiles, Structure and bonding (DCD model )

**$\eta^2$  alkyne transition metal compounds:** Introductions, preparation, chemical properties, Structure and bonding.  **$\eta^3$  allyl transition metal compounds:** Introduction, Structural verities in allyl transition metal compounds, General methods of preparation, chemical properties, structure and bonding.

**$\eta^4$  butadiene transition metal compounds:** Introduction, General methods of preparation, reaction on coordinated ligand, structure and bonding.  **$\eta^4$  Cyclobutadiene transition metal compounds:** Preparation and chemical properties of  $(C_4H_4)Fe(CO)_3$ , structure and bonding.

**$\eta^5$  Cyclopentadienyl transition metal compounds:** Introduction, classification of  $\eta^5$ - Cyclopentadienyl derivatives, Preparation and chemical properties of  $(\eta^5-C_5H_5)_2Mn$ ,  $(\eta^5-C_5H_5)Mn(CO)_3$ , structure and bonding in Ferrocene.

### Unit- IV: Organotransition metal compound as catalysts and synthetic reagents [12 hrs]

**Activation process:** consequent changes in the coordinated ligand reactivity, template effect.

**Protection:** Steric control, facilitation of nucleophilic addition reactions. **Product isolation:** Reductive elimination,  $\beta$ -eliminations, radical formation, alkene or arene displacement by

competing ligand, electron transfer from metal atom to an oxidant, release of carbenoid ligands.

**Unit -V: Catalytic processes involving organotransition metal compound: [12 Hrs]**

Hydrogenation of alkene using Wilkinson's catalysts, hydrosilation reaction, hydroformulation of alkene (oxo process) Ziegler Natta polymerizations. Fischer Tropsch process, water gas shift reaction. Monsanto process for acetic acid synthesis., Wacker process of oxidation of alkene.

**Reference Books:**

1. Organo metallic Chemistry, R. C. Mehrotra, & A. Singh
2. Principal and applications of organotransition metal Chemistry, J. P. Collman, L. S. Hegedus, J. R. Norton
3. Inorganic Chemistry , Attkin and Shriver
4. Advanced Inorganic Chemistry, Gurdeep Raj.
5. Inorganic Chemistry, J. E. Huhey

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## CHEEI-405: Polymer chemistry

04 Hrs/Week

Credits: 04

Marks : 100

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### **Unit-I: Fundamentals of Biological Macromolecules**

[12 hrs]

Chemical bonds in biological systems; Properties of water; Thermodynamic principles in biological systems; Properties and classification of amino acids; Structures of nucleic acids, Protein structure and function, Properties of nucleosides and nucleotides, Composition of nucleic acids, Electrophoresis, Factors affecting on Electrophoretic Mobility; Types of Electrophoresis; Free electrophoresis and Gel electrophoresis; Electrophoresis in genetic analysis; DNA Sequencing and DNA foot Printing.

### **Unit-II: Macromolecules**

[12 hrs]

Introduction, Formation of synthetic high polymers classification, Polymerization reactions: Chain and Step. Average molecular weight, Number average weight, Methods of determination of molar masses of polymers; Viscosity, Osmometry, Molar mass of charged macromolecules, Donnan membrane equilibrium, Ultracentrifugation, light scattering, Diffusion.

### **Unit-III: Chemistry of Polymerization**

[12 hrs]

Chain polymerization: free radical polymerization, ionic polymerization, co-ordination polymerization, Ziegler-Natta catalysts.

Step Polymerization: polycondensation, polyaddition, ring opening, electro chemical polymerization, group, Transfer polymerization, Polymerization techniques.

### **Unit-IV: Kinetics of Polymerization**

[12 hrs]

Free radical chain polymerization, Anionic polymerization, Cationic polymerization, Copolymerization, Free radical copolymerization, Ionic copolymerization, Copolycondensation.

### **Unit-V: Electronically Conducting Polymers**

[12 hrs]

Introduction, Theories of electronic conduction; Band theory of conduction, Hopping conduction, Super conduction, Mechanism of conduction, Doping mechanism, p-type, n-type, auto doping, Stimuli sensitive (smart) polymers, pH and temperature sensitive smart polymers, Applications: Photovoltaic devices, Sensors, LED and Solar cells, Electro chemical devices, Batteries etc.

### **Reference Books:**

1. Cantor, C. R. and Schimmel Biophysical Chemistry Vols. 1-3, W. H. Freeman (1980).

2. Lehninger, A.L., Nelson, D. L. and M. M. Lehninger, Principles of Biochemistry 4<sup>th</sup> Ed., W. H. Freeman (2004).
3. U. Satyanarayana; Biochemistry.
4. Upadhyay; Biophysical Chemistry.
5. L. Stryer, Biochemistry, 5<sup>th</sup> Edition, (2002) Freeman and Co. New York.
6. D. Voet, J. G. Voet, Biochemistry 3<sup>rd</sup> Edition (2004), Wiley International Publication.
7. D. L. Nelson and M. M. Cox, Lehninger Principles of Biochemistry 3<sup>rd</sup> Edition (2002) McMillan North Publication.
8. Polymer Science. By V. R. Gowariker, N. V. Viswnathan, Jayadev Sreedhar.
9. Polymers and Resins. By Brage Golding.
10. Electrical Properties of Polymers. By Tony Blythe and David Bloor.
11. Self doped conducting polymers. By Michael S. Freund and Bhavana Deore.
12. Polymer Science and Technology. By Premamoy Ghosh.

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## CHEEI-406 : Theoretical and structural inorganic chemistry

04 Hrs/Week

Credits : 04

Marks : 100

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### Unit- I: Applications of theoretical models to chemical compounds. [12 hrs]

**Valence bond model:** theoretical concept of hybridization, construction of wave functions for  $sp$ ,  $sp^2$ ,  $sp^3$ ,  $dsp^2$  and  $d^2sp^3$  hybridizations. Identification of nature of bonds. Application of VSEPER theory to covalent bonded anionic compounds.

### Unit- II: Crystal field theory [12 hrs]

Important feature of CFT, crystal field splitting d orbital in octahedral, tetrahedral, square planer and tetragonal complexes, factors affecting  $10Dq$ , application of CFT, CFSE and their uses, limitation of CFT

### Unit- III: Molecular orbital Theory [12 hrs]

Basic principles of MOT, linear combination of atomic orbitals, construction molecular orbital wave function of  $H_2$ ,  $H_2^+$ ,  $H_2^-$ . Molecular orbital energy level diagram of poly atomic molecules ( $NH_3$ ,  $BF_3$ ,  $BeH_2^-$ , octahedral and tetrahedral molecules).

Donor acceptor chemistry of  $NH_3$ :  $BF_3$ ,  $BF_3 : O(C_2H_5)_2$ ,  $Br_2 : CH_3OH$  adducts.  $\pi$ - Molecular orbitals of planer  $C_nH_n$  molecules, HOMO -LUMO energy, correlation of HOMO- LUMO energies with ionization energy, electron affinity, hardness and reactivity of molecules.

### Unit-IV: Chemical forces and its importance [12 hrs]

Types of chemical forces, covalent bonding, ionic bonding, dipole-dipole interaction, induced dipole interactions, dipole-induced dipole interactions, with suitable examples, interpretation of hydrogen bonding interactions in common organic compounds, solubility of ionic substances, ion solvent interactions with examples, Polarity of solvent, factors affecting the polarity of solvents, importance of polar and non polar solvent in chemical reactions.

### Unit -V: Chemistry of main group elements [12 hrs]

Synthesis, structure and properties of Borazines, phosphazenes and their polymers, Hetrocyclic inorganic systems, Sulfur- nitrogen chain and ring compounds, Xenon compounds, interhalogens compounds, Structural aspect of oxy acid of phosphorous, sulfur, nitrogen and halogens.

**Reference Books:**

1. Inorganic Chemistry - J E Huhey
2. Concept and models of Inorganic chemistry – Bodil E Douglas and Darl H
3. McDaniel , Oxford & IBH Pub. Co.
4. Inorganic chemistry- Gary L Miessler, Donald A Tarr 3<sup>rd</sup> Edn
5. Inorganic chemistry – Puri and Shrma
6. Inorganic chemistry – J D Lee
7. Inorganic chemistry- Attken
8. Quantum chemistry and spectroscopy- Engel
9. Physical chemistry - A molecular approach – Donald A Mc Quarrie , John D Simon

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**CHEIR-407 : Research project (Experimental)**

**24 Hrs/Week**

**Credits : 12**

**200 Marks**

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**CHEIR-408 : Research project (Dissertation, presentation and Seminars)**

**06 Hrs/week**

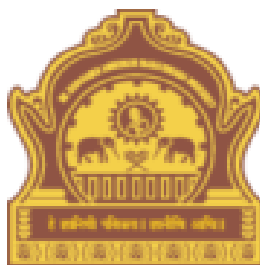
**Credits : 06**

**100 Marks**

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**DR. BABASAHEB AMBEDKAR MARATHWADA  
UNIVERSITY,  
AURANGABAD.**

**DEPARTMENT OF CHEMISTRY**



# **SYLLABUS**

**M. Sc. Organic Chemistry**  
**(Semester III & IV)**

**Choice Based Credit and Grading System**

**Effective from : June 2017**

The following will be the Choice Based Credit and Grading System structure of revised syllabus for M. Sc. III & IV semester Organic Chemistry effective from June 2017.

Semester	Paper Nos.	Title of Paper	Teaching (hr)/week	Marks	Credits
III- Semester	CHESC-301	Structural elucidation by spectral methods	04	100	04
	CHECO- 302	Organic synthesis	04	100	04
	CHECO- 303	Photochemistry, free radicals and pericyclic reactions	04	100	04
	CHEEO -304	Advanced organic chemistry OR	04	100	04
	CHEEO -305	Environmental chemistry OR	04	100	04
	CHEEO- 306	Green chemistry	04	100	04
	CHELO- 307	Laboratory course	06	50	03
	CHELO- 308	Laboratory course	06	50	03
	CHELO- 309	Laboratory course	06	50	03
IV semester	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

## CHESC-301: Structural elucidation by spectral methods

04 Hrs/Week

Credits: 04

Marks 100

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### **UNIT-I: Nuclear Magnetic Resonance Spectroscopy ( $^1\text{H}$ NMR) [12 hrs]**

Elementary ideas (Recapitulation); Spin-spin couplings, Different types of couplings, factors affecting on coupling constants, Karplus equation, Spin systems (AB, AX, ABX, AMX), Rate processes, spin decoupling, shift reagents, Nuclear Overhauser effect (NOE), INEPT and INADEQUATE.

### **UNIT-II: $^{13}\text{C}$ Nuclear Magnetic Resonance Spectroscopy [12 hrs]**

Elementary ideas, instrumental problems, chemical shifts (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbons); Effect of substituents on chemical shifts.

### **UNIT-III: Mass Spectroscopy [12 hrs]**

Introduction, ion production (EI, CI, FD and FAB), ion analysis, ion abundance, factors affecting on fragmentation, fragmentation of different functional groups, molecular ion peak, isotopic peaks, metastable peak, Nitrogen rule, McLafferty rearrangement, Retro-Diels-Alder reaction.

### **UNIT-IV [12 hrs]**

Problems based on joint applications of UV, IR,  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and Mass spectroscopy.

### **UNIT-V [12 hrs]**

**Mossbauer spectroscopy:** Principle, factors affecting the line position and shape, isomer effect and Quadrupole splitting iron salt like compounds, complexes, carbonyl compounds (temperature dependence of isomer shift and Quadrupole splitting in simple compound and coordination, polynuclear complexes), Numericals.

**Electron Spin Resonance Spectroscopy:** Principle of ESR spectroscopy, presentation of spectrum, hyperfine splitting in various structures, hyperfine splitting diagram of representative examples, factors affecting the magnitude of 'g' values, Zero field splitting, Kramer's degeneracy, Anisotropy in the hyperfine coupling constant, electron delocalization, instrumentation and applications.

### **Reference Books:**

1. Introduction to Spectroscopy: D. L. Pavia, G. M. Lampman, G. S. Kriz
2. Spectrometric Identification of Organic Compounds: R. M. Silverstein & F. X. Webster

3.  $^{13}\text{C}$  NMR Spectroscopy: G. C. Levy, R. L. Lichter, G. L. Nelson
4. Spectroscopic Methods in Organic Chemistry: D. H. Williams & I. Fleming
5. Absorption Spectroscopy of Organic Compounds: V. M. Parikh
6. Mass Spectrometry: K. G. Das & James
7. Coordination Chemistry by Experimental Methods: K. Barger
8. Coordination Chemistry vol. I: E. Martell
9. Physical Methods for Chemistry: R. S. Drago
10. Structural Methods in Inorganic Chemistry: E. A. V. Ebsworth & D. W. H. Rankin
11. Organic Structure Analysis: Philips Crews

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## CHECO-302: Organic synthesis

04 Hrs/Week

Credits: 04

Marks 100

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### UNIT-I Oxidation

[12 hrs]

(a) Oxidation of alcohol to aldehyde, ketone or acid: Jones reagent, Swern oxidation, Collins reagent, Fetizon's reagent, PCC, PDC, PFC, IBX, Activated  $\text{MnO}_2$ , Chromyl chloride (Etard reaction), **TEMPO, CAN, NMO, Moffatt oxidation**

(b) Oxidative cleavage of Carbon-Carbon double bonds:  $\text{KMnO}_4$ , Ozonolysis.

(c) Oxidations using  $\text{SeO}_2$ , **PhSeBr**.

**(d) Selective cleavages at functional groups: Cleavage of glycols,  $\text{IO}_4^-$ ,  $\text{Pb}(\text{OAc})_4$ .**

### UNIT-II Reductions

[12 hrs]

(a) Catalytic Hydrogenation; (b) Reduction of nitriles, oximes and nitro compounds; (c) Reduction of acids and Esters; (d) Reduction with metal hydride- Sodium cyanoborohydride, Diborane, L- & K-Selectrides,  $\text{LiBH}_4$ , DIBAL-H; (e) Birch reduction and related reactions, (h) Luche reagent, Wolf-Kishner reduction, Clemmenson reduction, Wilkinson catalyst, TBTH.

### UNIT-III Organic Reagents

[12 hrs]

DCC, EDC, DDQ, 1,3 Dithiane, LDA, DMDO,  $\text{OsO}_4$ ,  $\text{RuO}_4$ ,  $\text{SmI}_2$ , Dess-Martin Periodinane, Diazomethane, Lawesson's reagent.

### UNIT-IV

[12 hrs]

#### (A) Ylides and Enamines

(i) Ylides: Preparation and their synthetic applications along with their stereochemical aspects of Phosphorous, Sulphur and Nitrogen ylides.

(ii) Enamines: Generation & application in organic synthesis with mechanistic pathways, stork enamine reaction.

#### **(B) Rearrangements**

**Pummerer, Payne, Eschenmoser fragmentation, Brook, Wagner-Meerwein, Wolf, Semipinacol, Epoxide rearrangement with lewis acid, Dienone-Phenol rearrangement, Tiffeneau-Demjanov, Favorskii, von Richter, Wittig, Neber, Smiles, Fries, Curtius, Lossen, Schmidt, Steven, Hofmann, Iodolactonisation.**

### **UNIT-V Formation of Carbon-Carbon bonds via organometallic reagents [12 hrs]**

Synthesis and applications of organo Lithium, Magnesium, Titanium, Cerium, Copper, Chromium, Zinc, Boron, Silicon, Cadmium

**Reference Books:**

1. Organic Chemistry: Clayden, Greeves, Warren and Wothers
2. Stereochemistry of Organic Compounds (Principle and application): D. Nasipuri
3. Stereochemistry of Organic compounds: Ernest L. Eliel / Samuel H. Wilen
4. Organic Synthesis: W. Carruthers
5. Organic Reagents: Fieser & Fieser
6. Organic Synthesis: M. B. Smith
7. Advanced Organic Chemistry; Part A and B: F. A. Carey & R. J. Sundberg
8. Modern Organic Synthesis: An Introduction: G. S. Zweifel & M. H. Nantz
9. A Guidebook To Mechanism In Organic Chemistry: Peter Sykes
10. Organic Synthesis Concepts, Methods, Starting Materials: J. Fuhrhop, G. Penzlin
11. Organic Chemistry: An Intermediate Text: Robert V. Hoffmann
12. Advanced Organic Chemistry: Jerry March
13. Organic Synthesis: R. O. C. Norman and Coxan
14. Name Reactions: Jie Jack Li

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**CHECO-303: Photochemistry, free radicals and pericyclic reactions**

**04 Hrs/Week**

**Credits: 04**

**Marks 100**

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**UNIT-I: Pericyclic Reactions-I**

**[12 hrs]**

Features and classification of pericyclic reactions, Phases, nodes and symmetry properties of molecular orbital in ethylene, 1,3-butadiene, 1,3,5-hexatriene. Allyl cation, allyl radical, pentadienyl cation and pentadienyl radical. Thermal and photochemical reactions.

**Electrocyclic reactions:** Woodward-Hoffmann selection rules for electrocyclic reactions. Explanation for the mechanism of electrocyclic reactions by: (i) Symmetry properties of HOMO of open chain partner; (ii) Conservation of orbital symmetry and orbital symmetry correlation diagram and (iii) Huckel-Mobius aromatic and antiaromatic transition state method.

**UNIT-II: Pericyclic Reactions-II**

**[12 hrs]**

**Cycloaddition reactions:** Diels-Alder reaction. Woodward-Hoffmann selection rules for cycloaddition reactions. Explanation for the mechanism of cycloaddition reactions by 1) Conservation of orbital symmetry and orbital symmetry correlation diagrams 2) Fukui Frontier Molecular Orbital (FMO) theory and (3) Huckel-Mobius aromatic and antiaromatic transition state method. Endo-exo selectivity in Diels-Alder reaction and its explanation by FMO theory. Examples of cycloaddition reactions.

**Sigmatropic reactions:** Selection rules for [i,j] shifts. Cope, degenerate Cope and Claisen rearrangements. Explanation of sigmatropic reactions by (i) symmetry properties of HOMO (ii) Huckel-Mobius aromatic and antiaromatic transition state method. Introduction to chelotropic reactions and the explanation of mechanism by FMO theory.

**UNIT-III: Photochemistry-I**

**[12 hrs]**

**Photochemistry of ( $\pi$ ,  $\pi^*$ ) transitions:** Excited state of alkenes, cis-trans isomerisation, photochemistry state, electrocycloaddition and Sigmatropic rearrangements, di  $\pi$ -methane rearrangement.

**Intermolecular reactions:** photocycloadditions, photodimerisation. Photoaddition reactions. Excited states of aromatic compounds, photodimerisation of benzene, photosubstitution reactions of aromatic compounds and Photo-Fries rearrangement.



**UNIT-IV: Photochemistry-II****[12 hrs]**

**Photochemistry of (n,  $\pi^*$ ) transitions:** Excited state of carbonyl compounds, Norrish-I and Norrish-II

**Addition to C-C multiple bonds:** Paterno-Buchi reaction, photochemistry of alkyl peroxides, hypohalites and nitriles. Barton reaction. Photochemistry of azo compounds, diazo compounds, azides and diazonium salts. Singlet oxygen-photo oxygenation reactions. Ene reaction, formation of dioxetanes and endoperoxides. Chemiluminescent reactions. Oxidative coupling.

**UNIT-V: Free radical reactions****[12 hrs]**

Introduction, generation, stability, reactivity, characteristics, structural and stereo chemical properties of free radicals, Persistent free radicals.

**Reaction of free radicals:** Addition, substitutions, fragmentations, Oxidations and reductions, Detection of free radicals, Homolysis and free radical displacement. Radical chain reactions, Addition and rearrangements, radical cyclization, reactivity of aliphatic and aromatic substrates at bridgehead, Coupling of alkynes and arylation of aromatic compound by diazonium salt, Sandmeyer reaction, Hunsdieker reaction, Allylic halogenations, McMurry reaction, Acyloin condensation, Birch reduction, Bouveault-Blank reduction.

**Reference Books:**

1. Advanced Organic Chemistry Part A & Part B: F. A. Carey & R. J. Sundberg
2. Advanced Organic Chemistry: Jerry March
3. Organic Chemistry: Clayden, Greeves, Warren & Wothers.
4. Organic Chemistry: Stanley H. Pine
5. Organic Synthesis: W. Carruthers
6. Organic Synthesis: Norman and Coxon

**CHEEO-304: Advanced organic chemistry**

**04 Hrs/Week**

**Credits: 04**

**Marks 100**

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**UNIT-I: Introduction to Bioorganic chemistry**

**[12 hrs]**

Basic concepts, Proximity effects in organic chemistry, Molecular adaptation, Molecular recognition.

**UNIT-II: Enzyme Chemistry**

**[12 hrs]**

Introduction, Nomenclature, Classification and Extraction of enzymes, Introduction to catalysis and enzymes; Multifunctional catalysis, Intramolecular Catalysis, Mechanism of enzyme action, Factors responsible for enzyme specificity, Enzyme activity and kinetics (Michaelis Menten and Lineweaver–Burk plots), Enzyme Inhibitions (Reversible and irreversible), Structure, Mechanism of action and applications of  $\alpha$ -Chymotrypsin, Ribonuclease, lysozyme and Carbopeptidase-A. Enzymes in synthetic organic chemistry. [Additions, eliminations, substitutions, condensations, cyclocondensations, oxidations, reductions and rearrangement reactions are to be covered]

**UNIT-III: Co-Enzyme Chemistry**

**[12 hrs]**

Chemical structures of co-enzymes and cofactors, Oxidoreduction ( $\text{NAD}^+$ ,  $\text{NADP}^+$ ), Pyridoxal phosphate (PLP), Thiamine pyrophosphate (TPP), Biotin ( $\text{CO}_2$  carrier), Haemoglobin ( $\text{O}_2$ -carrier), Flavin (FMN, FAD,  $\text{FADH}_2$ ), Oxene Reactions, Lipoic acid, Mechanisms of reactions catalyzed by co-factors.

**UNIT-IV: Asymmetric Synthesis**

**[12 hrs]**

Chiral pool, Chiral auxiliary, Enantio- & Diastereoselective synthesis, Chiral reagent and chiral catalyst including CBS reagent, NADH, Asymmetric hydrogenation including BINAP, Hydroboration-  $\text{Ipc}_2\text{BH}$ ,  $\text{IpcBH}_2$ , Asymmetric epoxidation- (+) DET & (-) DET, Sharpless, Jacobson, Asymmetric dihydroxylation-  $(\text{DHQD})_2\text{PHAL}$  &  $(\text{DHQ})_2\text{PHAL}$ , Felkin-Anh model, Zimmermann-Traxler transition state model, Proline catalyzed asymmetric reactions.

**UNIT-V: Name Reactions**

**[12 hrs]**

Arndt-Eistert, Hunsdiecker reaction, Baeyer-Villiger, Dakin, Gabriel synthesis, Michael, Darzen, Prins, Henry, Reimer-Tiemann, Hoffmann–Löffler–Freitag, Dieckmann cyclization, Chichibabin, Vilsmeier, Ene, Ullmann reaction, Mannich, Strecker amino acid synthesis.

Bamford-Steven, Baylis-Hillmann, Corey-Fuchs Reaction, Julia olefination, Mukaiyama aldol, Mitsunobu, Peterson olefination, Corey-Winter olefination, Woodward and Prevost dihydroxylation, Shapiro, Ritter, Stille, Heck, Sonogashira, Suzuki, Duff, Chugaev, Petasis, McMurry reaction and Coupling. Ring closing metathesis (Grubb's metathesis), Aldol-Tishchenko (Evans-Tishchenko reaction), Ugi, Passerini, Biginelli, Hantzsch condensation.

**Reference Books:**

1. Bioorganic chemistry (A chemical approach to enzyme action): Hermann Dugas.
2. Biotransformation in Organic chemistry: K. Faber
3. Enzyme structure and Mechanism: Alan Fersht.
4. Enzyme catalysis in organic synthesis vol.1: Karlheinz Drauz and Herbert Waldmann.
5. Bioorganic, Bioinorganic and supramolecular chemistry: P. S. Kalsi and J. P. Kalsi.
6. Organic chemistry IV<sup>th</sup> Edn.: G. Marc Loudon.
7. Stereochemistry of Organic Compounds (Principle and application): D. Nasipuri
8. Stereochemistry of Organic compounds: Ernest L. Eliel / Samuel H. Wilen
9. Advanced Organic Chemistry; Part A and B: F. A. Carey & R. J. Sundberg
10. Organic Chemistry: Clayden, Greeves, Warren and Wothers
11. Organic Synthesis: W. Carruthers
12. Organic Synthesis: M. B. Smith
13. Name Reactions: Jie Jack Li
14. Name Reactions and Reagents in Organic Synthesis: B. P. Mundy, M. G. Ellerd, F. G. Favalaro

## CHEEO-305: Environmental chemistry

04 Hrs/Week

Credits: 04

Marks 100

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### UNIT-I: Introduction to Environmental Chemistry

[12 hrs]

Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments, The natural cycles of environment (Hydrological, Oxygen, Nitrogen)

### UNIT-II: Atmosphere, Hydrosphere and Lithosphere

[12 hrs]

**Atmosphere:** Regions of the atmosphere, Reactions in atmospheric chemistry, Earth's radiation balance, Particles, ion and radicals in atmosphere; Chemistry of ozone layer.

**Hydrosphere:** Complexation in natural water and waste-water, Micro-organisms in aquatic chemical reactions, Eutrophication, Microbiology mediated redox reactions.

**Lithosphere:** Inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and NPK in soil.

### UNIT-III: Chemical Toxicology

[12 hrs]

Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur oxides.

### UNIT-IV: Air Pollution

[12 hrs]

Particulates, Aerosols, SO<sub>x</sub>, NO<sub>x</sub>, CO<sub>x</sub> and hydrocarbon, Photochemical smog, Air-quality standards

### UNIT-V: Water Pollution

[12 hrs]

Water-quality parameters and standards: physical and chemical parameters, Dissolved oxygen, BOD, COD, Total organic carbon, Total nitrogen, Total sulfur, Total phosphorus and Chlorine, Chemical speciation (Pb, As, Hg)

### Reference Books:

1. G.W. Vanloon, S.J. Duffer, Environmental Chemistry - A Global Perspective, Oxford University Press (2000).
2. F.W. Fifield and W.P.J. Hairens, Environmental Analytical Chemistry, 2nd Edition (2000), Black Well Science Ltd.
3. Colin Baird, Environmental Chemistry, W.H. Freeman and Company, New York (1995).
4. A.K. De, Environmental Chemistry, 4th Edition (2000), New Age International Private Ltd., New Delhi.
5. Peter O. Warner, Analysis of Air Pollutants, 1st Edition (1996), John Wiley, New York.
6. S.M. Khopkar, Environmental Pollution Analysis, 1st Edition (1993), Wiley Eastern Ltd., New Delhi.
7. S.K. Banerji, Environmental Chemistry, 1st Edition (1993), Prentice-Hall of India, New Delhi.

**UNIT-I: Introduction to Green Chemistry**

Green chemistry, relevance and goals, Anastas' twelve principles of green chemistry-Tools of green chemistry: alternative starting materials, reagents, catalysts, solvents and processes with suitable examples.

**UNIT-II: Microwave mediated organic synthesis (MAOS):**

Microwave activation, advantage of microwave exposure, specific effects of microwave, Neat reactions, solid supports reactions, Functional group transformations, condensations reactions, oxidations, reductions reactions, multi-component reactions.

**UNIT-III: Ionic liquids and PTC**

Introduction, synthesis of ionic liquids, physical properties, applications in alkylation, hydroformylations, epoxidations, synthesis of ethers, Friedel-craft reactions, Diels-Alder reactions, Knoevenagel condensations, Wittig reactions, Phase transfer catalyst, Synthesis, applications.

**UNIT-IV: Supported catalysts and bio-catalysts for Green chemistry**

Introduction, the concept of atom economy, supported metal catalysts, mesoporous silicas, the use of Biocatalysts for green chemistry, modified bio catalysts, fermentations and biotransformations, fine chemicals by microbial fermentations, vitamins and amino acid, Baker's yeast mediated biotransformations, Biocatalyst mediated Baeyer-Villiger reactions.

**UNIT-V: Supramolecular Chemistry and Biomimetic Chemistry**

Host-Guest approach, Chiral recognition, Ionophores, Crown ethers, cryptands, Micelles, Cyclodextrins, calixarenes.

**Reference Books**

1. Green Chemistry-Environmentally benign reactions. V. K. Ahluwalia. Ane Books India (Publisher).
2. Green Chemistry-Designing Chemistry for the Environment. Paul T. Anastas & Tracy C. Williamson.
3. Green Chemistry-Frontiers in benign chemical synthesis and processes. Paul T. Anastas & Tracy C. Williamson.
4. Green Chemistry- Environment friendly alternatives. Rashmi Sanghi & M. M. Srivastava

**CHELO-307: Laboratory course**

**06Hrs/Week**

**Credits: 03**

**Marks : 50**

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Qualitative analysis of ternary mixtures.

In a mixture at least one liquid one water soluble compound be given.

**CHELO-308: Laboratory course**

**06 Hrs/Week**

**Credits: 03**

**Marks : 50**

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Preparations involving at least two stage based on name reactions, condensations, cyclocondensations, reagents and rearrangements (as covered under the theory). Separation purification of the product by column is desired.

**CHELO-309: Laboratory course**

**06 Hrs/Week**

**Credits: 03**

**Marks : 50**

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(A) Preparations involving one stage based upon the green synthetic protocols (as covered in theory syllabus).

(B) Structure elucidation of organic compounds by spectral analyses.

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## CHECO-401 : Heterocyclic chemistry

02 Hrs/Week

Credits: 02

Marks 50

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### UNIT-I

[12 hrs]

Nomenclatures of all types of heterocycles, Classification of heterocycles: as aromatics based upon various membered ring systems.

### UNIT-II

[18 hrs]

General synthetic routes based on name reactions, reactivities, utilities and wherever possible spectral analyses of the following class of heterocycles.

**Four membered:** Azetidines, including  $\beta$ - lactams.

**Five membered:** Thiazoles, Oxazoles, Pyrazoles and Imidazoles.

**Six membered:** Pyridines, Pyrimidines.

**Fused heterocycles:** Flavones, Chromones, Coumarines, Indoles, Quinolines, Benzodiazepines, and Phenothiazines.

### Reference Books:

1. Heterocyclic Chemistry: vol. I, II, III: R. R. Gupta, M. Kumar and M. Gupta
2. Heterocyclic Chemistry: Joules and Mills
3. Modern heterocyclic Chemistry: L. A. Paquette (Benjamin)
4. Organic Chemistry: Jonathan Clayden

## CHECO-402: Organic synthesis: Retrosynthetic approach

04 Hrs/Week

Credits: 04

Marks 100

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### UNIT-I Disconnection Approach

[18 hrs]

Introduction to:

- (i) Grounding of organic chemistry for understanding retrosynthesis;
- (i) Retrosynthetic analysis and designing of the synthesis;
- (ii) Disconnection approach: An introduction to synthons, synthetic equivalents, disconnection approach, functional group interconversions, importance of order of events in organic synthesis, one and two group C-X disconnections, selective organic transformations: chemoselectivity, regioselectivity, stereoselectivity, enantioselectivity, Reversal of polarity, cyclization reactions, amine synthesis.

### UNIT-II Protecting Groups

[06 hrs]

Protection and deprotection of hydroxyl, carbonyls in aldehydes and ketones, amines, carboxylic acids, alkenes and alkynes.

### UNIT-III C-C Disconnections

[12 hrs]

#### (i) One group C-C Disconnections:

Alcohols (including stereoselectivity), carbonyls (including regioselectivity), Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

#### (ii) Two group C-C Disconnections:

Diels-Alder reactions, 1,3 difunctionalized compounds and  $\alpha$ ,  $\beta$ -unsaturated compounds, control in carbonyl condensations, 1,5 difunctionalized compounds, Michael addition and Robinson annelation.

### UNIT-IV Ring Synthesis

[12 hrs]

Introduction to ring synthesis, saturated heterocycles, synthesis of 3, 4, 5 and 6 membered rings, rearrangements and photochemistry in synthesis, aromatic heterocycles.

### UNIT-V Complex molecules

[12 hrs]

Synthetic routes based on retrosynthetic analysis for following molecules: Longifoline, Reserpine, Juvabione, Aphidicoline, Taxol.

#### Reference Books:

1. Organic Synthesis: The Disconnection Approach: Stuart Warren
2. Designing Organic Synthesis: Stuart Warren



3. Organic Synthesis: Strategy and Control: Paul Wyatt and Stuart Warren
4. The Logic of Chemical Synthesis: E. J. Corey and Xue-Min Chelg
5. Classics in Total Synthesis I, II and III: K. C. Nicolaou and others
6. Organic Synthesis Concepts, Methods, Starting Materials: J. Fuhrhop, G. Penzlin
7. Some Modern Methods of Organic Synthesis: W. Carruthers
8. Organic Synthesis: M. B. Smith
9. Principles of Organic Synthesis: R. Norman and J. M. Coxan.
10. Advanced Organic Chemistry: Jerry March
11. Organic Chemistry: Clayden, Greeves, Warren and Wothers

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## CHECO-403: Chemistry of natural products

04 Hrs/Week

Credits: 04

Marks 100

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### UNIT-I: Terpenoids & Carotenoids

[12 hrs]

Classification, Nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule, Structure determination, stereochemistry, and synthesis of the following representative molecules: Citral, Geraniol,  $\alpha$ -Terpineol, Menthol, Farnesol, Zingiberene, Phytol, Abietic acid and  $\beta$ - Carotene.

### UNIT-II: Alkaloids

[12 hrs]

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry and synthesis of the following: Ephedrine, (+)-coniine, nicotine, atropine, Quinine and Morphine.

### UNIT-III: Steroids

[12 hrs]

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Bile acids, Androsterone, Testosterone, Estrone, Progesterone.

### UNIT-IV: Anthocyanins and Flavones

[12 hrs]

Occurrence, nomenclature and general methods of structure determination. Synthesis of cyanidin chloride, cyanin, Hirsutidin chloride, Flavones (Kostanecki and Baker-Venkataraman approaches), Flavonols, Quercetin, and Isoflavones.

### UNIT-V: Biogenesis

[12 hrs]

The building blocks and construction mechanisms of the following:

- (a) Terpenoids: Mono-, Sesqui-, Di-, Tri-Terpenoids and steroids.
- (b) Alkaloids: pyridine alkaloids, Benzyl Isoquinoline alkaloids, morphine alkaloids and Indole alkaloids.
- (c) The Shikimic acid pathway.

### Reference Books:

1. The Organic Chemistry of Drug Design and Drug Action: R. B. Silverman, Academic press.
2. Natural Products: Chemistry and Biological Significance: J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthrope and J. B. Harborne, Longman, Essex.

3. Organic Chemistry: Vol. II, I. L. Finar, ELBS.
4. Introduction to Flavonoids: B. A. Bohm, Harwood Academic Publishers
5. New Trends in Natural Product Chemistry: Atta-ur-Rahman and M. I. Choudhary, Harwood Academic publishers.
6. Biogenesis of Natural Products: Baldev Kumar and Harishkumar Chopra (Narosa Publication)

## CHEEO-404: Medicinal chemistry

04 Hrs/Week

Credits: 04

Marks 100

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### UNIT-I: Basic consideration of drug activity

[18 hrs]

Definition and Introduction of following terms-Drug, Prodrug, Hard and Soft drugs, agonists, antagonists, affinity, efficacy, potency, isosterism, bioisosterism, pharmacophores, lead molecule, lethal dose (LD50) and effective dose (ED50) (i) Factors affecting bioactivity, (ii) Theories of drug activity, (iii) Structure activity relationship (SAR), QSAR (2D and 3D method) and Hantzsch equation (iv) Drug receptor mechanism.

### UNIT-II Pharmacokinetics

[06 hrs]

- (i) Drug absorption, Distribution and deposition of drugs.
- (ii) Excretion and elimination of drugs, Bioavailability.

### UNIT-III Pharmacodynamics

[12 hrs]

- (i) Mechanism of drug action: Enzyme stimulation and enzyme inhibition, antimetabolites, membrane active drugs, chelation; (ii) Drug metabolism and inactivation: Factors affecting drug metabolism, pathways of drug metabolism [Metabolic reaction (Phase I) and conjugation reaction (Phase II)].

### UNIT-IV Classification of Drugs

[06 hrs]

The detail contents of the each class of the drugs.

### UNIT-V

[18 hrs]

Synthesis and Utilities of the following drug molecules (at least one convenient synthetic route with possible mechanism) from following classes:

**I. Anti inflammatory Drugs:** (a) Naproxen (b) Ibuprofen (c) Oxaprozin (d) Diclofenac Sodium (e) Rofecoxib (f) Celecoxib.

**II. Anti-hypertensive Drugs:** (a) Verapamil (b) Captopril (c) d-sotalol (d) Atenolol (e) Diltiazem (f) Semotiadil fumarate.

**III. Drugs acting on CNS:** (a) CNS Stimulant : Dextro-amphetamine

(b) Respiratory Stimulant : Doxapram

(c) CNS anti-depressant : (i) Chlorpromazine (Antipsychotic) (ii) Diazepam (Anxiolytic)

(iii) Phenobarbitol (Antiepileptic)

#### **IV Anesthetic Drugs:**

(a) General : Ketamine (b) Local : (i) Lidocaine (ii) Procaine

**V. Antibiotics:** (a) Chloramphenicol (b) Ampicillin (c) Amoxicillin (d) Cefepime (e) Cefpirome

(f) Antimycobacterial: Ethambutol (g) Antiviral: Acyclovir (h) Antimicrobial: Sulfamethoxazole

**VI. Antidiabetics :** (a) Troglitazone (b) Chlorpropamide (c) Tolbutamide

**VII. Antineoplastic Drugs:** (a) Antagonist: Fluorouracil (b) Alkylating agents: i) Chlorambucil

(ii) Cis-Platin

#### **Reference Books:**

1. FOYE'S Principles of Medicinal Chemistry VIth Edition: Thomas L. Lemke, David A. Williams, Victoria F. Roche and S. William Zito.
2. Introduction of Medicinal Chemistry: A. Gringuage, Wiley-VCH.
3. Synthesis of Essential Drugs: R. S. Vardanyan and V. J. Hruby.
4. Volumes of Burger's Medicinal Chemistry: M. E. Wolf, JohnWiley.
5. Medicinal Chemistry: David J. Triggle.
6. Essentials of Medicinal Chemistry IInd: Andrejus Korolkovas, WileyVCH.

## CHEEO-405 : Organic high polymers

04 Hrs/Week

Credits: 04

Marks 100

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### UNIT-I: Introduction to Polymers

[12 hrs]

- (i) Introduction to organic polymers and various terms like Monomer, comonomer, mesomer, homopolymer, heteropolymer, co-polymer, degree of polymerization, plastic, resin, fibers et
- (ii) Mechanism of polymerizations (Chain and condensation) and methods of polymerizations viz. mass, solution, emulsion and suspension.

### UNIT-II: Evaluation of Polymers

[12 hrs]

Molecular weight of polymers and their determinations by end group analysis, sedimentation, osmometric and viscometric measurements.

### UNIT-III: Natural Polymers

[12 hrs]

Isolations, characterizations and regenerations/derivatizations of natural polymers like Cellulose, Rubber and natural silk/ wool.

### UNIT-IV: Synthetic Polymers

[18 hrs]

Mechanism of polymerization, reactivity, stability, and applications of following polymers:

Polyethylene, polypropylene, polyvinyl chloride, polyvinyl acetate, and polymethyl methacrylate.

Polyethylene terphthalate, alkyd resin, polycarbonate and nylons.

Phenoplast, urea- formaldehyde resin, melamine-formaldehyde resin, polyurethanes, polysiloxane and epoxy resins

### UNIT-V: Processing of Polymeric Materials

[06 hrs]

Molding, Fiber formation, formation of films, fillers, plasticizers and cross linking agents

### Reference Books:

1. Textbook of Polymer Science: Fred W. Billmeyer.
2. Polymer Science: V. R. Gowarikar, N. N. Viswanathan, Jaydeep Sreedhar
3. Organic Polymer Chemistry: K. J. Saunder

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## CHEEO-406 : Drug design and drug discovery

04 Hrs/Week

Credits: 04

Marks 100

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### UNIT-I: Principles of Drug design and drug discovery

[12 hrs]

Introduction to drug discovery, Folklore drugs, stages involved in drug discovery- disease, drug targets, bioassay. Discovery of a lead, screening of natural products and synthetic compound libraries. Pharmacokinetics (ADME), pharmacodynamics, Nature of drug-receptor interactions and their theories-Occupancy theory, Induced-fit theory, Macromolecular perturbation theory and Two-state model of receptor activation. Natural products as lead structures in drug discovery, Pharmacophore, structure pruning technique e.g. morphine. Discovery of lead structure from natural hormones and neurotransmitters, Principles of design of agonists (e.g. Salbutamol), antagonists (e.g. cimitidine) and enzyme inhibitors (e.g. captopril), Drug discovery without lead, serendipity, Penicillin and Librium as examples, Principles of prodrug design.

### UNIT-II: Lead modification and SAR Studies

[12 hrs]

**SAR:** Lead modification strategies, Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead. Discovery of oxaminquine, salbutamol, cimitidine and captopril SAR studies in sulfa drugs, benzodiazepines, and taxol analogs.

### UNIT-III: Quantitative Structure-Activity Relationship (QSAR) studies

[12 hrs]

Introduction, physicochemical properties - pKa, electronic effects and Hammett constants ( $\sigma$ ), lipophilicity constant ( $\pi$ ), steric effects and Taft's constant, linear and nonlinear relationship between biological activity and Hammett/ Lipophilicity Substituent constants. Lipinski rule of five. Hansch analysis, Craig's plot, Topliss scheme, Free Wilson approach, cluster significant analysis. Principles of molecular modeling in drug design.

### UNIT-IV: Combinatorial Synthesis

[12 hrs]

Introduction, Combinatorial approach, Combinatorial libraries, technologies. Solid phase synthesis, types of resins, Linkers, Reactants for solid phased synthesis, Methods of Parallel synthesis: Haughton's tea bag procedure, Automated parallel synthesis. Methods in Mixed combinatorial synthesis: general principles. Furkasmix and split combinatorial synthesis, Structure determination of active compounds, Deconvolution, Methods in deconvolution-recursive deconvolution, tagging and use of decoded sheets. Examples of Combinatorial

Chemistry, Planning and designing of combinatorial synthesis, Spider like scaffolds, drug molecules, Automation in Combinatorial chemistry, High throughput screening.

### Reference books

1. Burger's medicinal chemistry and drug discovery by Manfred E. Wolf.
2. Introduction to Medicinal chemistry by Patrick.
3. Introduction to drug design by R Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. by William Foye
6. Biochemical approach to medicinal chemistry by Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
8. Drug design by E.J.Arienes
9. Principles of Medicinal Chemistry Vol I & II by Kadam et al
10. Medicinal chemistry An introduction by Garreth Thomas
11. Organic and Pharmaceutical chemistry By Delgrado
12. Organic Pharmaceutical chemistry By Harikishan singh
13. Medicinal Chemistry By Ashtoshkar
14. Medicinal Chemistry By Chatwal
15. Organic Drug synthesis By Ledneicer Vol 1-6
16. Strategies for organic drug synthesis and design By Daniel Ledneicer.
17. Top Drugs: Top synthetic routes By John Saunders
18. Burger's Medicinal Chemistry and Drug Discovery: Principles and Practices. Vol. 1.
19. Medicinal Chemistry by G. Patricks.
20. Text book of Drug Design and Discovery, Edited by Povl Krogsgaard – Larsen Tommy Liljefors.



**CHEOR-407: Research project (Experimental)**

**24 Hrs/week**

**Credit : 12**

**200 Marks**

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**CHEOR-408 : Research project (Dissertation, Presentation and Seminars)**

**6 Hrs/week**

**Credit : 6**

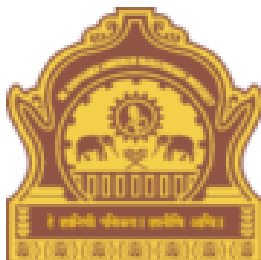
**100 Marks**

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**DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY,  
AURANGABAD.**

**DEPARTMENT OF CHEMISTRY**



# **SYLLABUS**

**M. Sc. Physical Chemistry**

**(Semester III & IV)**

**Choice Based Credit and Grading System**

**Effective from : June 2017**

The following will be the Choice Based Credit and Grading System structure of revised syllabus for M. Sc. III & IV semester Physical Chemistry effective from June 2017.

Semester	Paper Nos.	Title of Paper	Teaching (hr)/week	Marks	Credits
III- Semester	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 , <b>OR</b>	04	100	04
	CHEEP -305	Environmental chemistry, <b>OR</b>	04	100	04
	CHEEP-306	Nuclear chemistry	04	100	04
	CHELP-307	Laboratory course	06	50	03
	CHELP-308	Laboratory course	06	50	03
	CHEPR-309	Laboratory course	06	50	03
IV semester	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	Nano chemistry , <b>OR</b>	04	100	04
	CHEEP -405	Instrumental methods of chemical analysis, <b>OR</b>	04	100	04
	CHEEP-406	Biophysical chemistry	04	100	04
	CHEPR - 407	Research project (Experimental)	24	200	12
	CHEPR - 408	Research project (Dissertation Presentation and Seminars)	06	100	06

## CHESC-301: Structural elucidation by spectral method

04 Hrs/Week

Credits: 04

Marks 100

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### UNIT-I: Nuclear Magnetic Resonance Spectroscopy ( $^1\text{H}$ NMR)

[12hrs]

Elementary ideas (Recapitulation); Spin-spin couplings, Different types of couplings, factors affecting on coupling constants, Karplus equation, Spin systems (AB, AX, ABX, AMX), Rate processes, spin decoupling, shift reagents, Nuclear Overhauser effect (NOE), INEPT and INADEQUATE.

### UNIT-II: $^{13}\text{C}$ Nuclear Magnetic Resonance Spectroscopy

[12hrs]

Elementary ideas, instrumental problems, chemical shifts (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbons); Effect of substituents on chemical shifts.

### UNIT-III: Mass Spectroscopy

[12hrs]

Introduction, ion production (EI, CI, FD and FAB), ion analysis, ion abundance, factors affecting on fragmentation, fragmentation of different functional groups, molecular ion peak, isotopic peaks, metastable peak, Nitrogen rule, McLafferty rearrangement, Retro-Diels-Alder reaction.

### UNIT-IV

[12hrs]

Problems based on joint applications of UV, IR,  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and Mass spectroscopy.

### UNIT-V

[12hrs]

**Mossbauer spectroscopy:** Principle, factors affecting the line position and shape, isomer effect and Quadrupole splitting iron salt like compounds, complexes, carbonyl compounds (temperature dependence of isomer shift and Quadrupole splitting in simple compound and coordination, polynuclear complexes), Numericals. **Electron Spin Resonance Spectroscopy:** Introduction, principle of ESR spectroscopy, presentation of spectrum, hyperfine splitting in various structures, hyperfine splitting diagram of representative examples, factors affecting the magnitude of 'g' values, Zero field splitting, Kramer's degeneracy, Anisotropy in the hyperfine coupling constant, electron delocalization, instrumentation and applications.

### Reference Books:

1. Introduction to Spectroscopy: D. L. Pavia, G. M. Lampman, G. S. Kriz
2. Spectrometric Identification of Organic Compounds: R. M. Silverstein & F. X. Webster
3.  $^{13}\text{C}$  NMR Spectroscopy: G. C. Levy, R. L. Lichter, G. L. Nelson

4. Spectroscopic Methods in Organic Chemistry: D. H. Williams & I. Flemming
5. Absorption Spectroscopy of Organic Compounds: V. M. Parikh
6. Mass Spectrometry: K. G. Das & James
7. Coordination Chemistry by Experimental Methods: K. Barger
8. Coordination Chemistry vol. I: E. Martell
9. Physical Methods for Chemistry: R. S. Drago
10. Structural Methods in Inorganic Chemistry: E. A. V. Ebsworth & D. W. H. Rankin
11. Organic Structure Analysis: Philips Crews

## CHECP-302: Solid state chemistry

04 Hrs/Week

Credits: 04

Marks 100

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### Unit-I: Solid State Reactions

12 Hrs

General Principles, Classification, Wagner reaction mechanism, Laws governing nucleation, Growth of nuclei, improving reactivity of solids, co precipitation as a precursor to solid state reactions, Kinetics of solid state reactions, factors affecting the reactivity of solid state reactions. General principles of growing single crystals, General conditions for crystal growth, solvent properties and saturated solutions, methods for growing crystals, slow evaporation, slow cooling, variation on slow evaporation and slow cooling, solvent diffusion, reactant diffusion, sublimation and seed crystals.

### Unit-II: Imperfections in solids

12 Hrs

Perfect and imperfect crystal, Point defects, Stiochiometric defects, Schottky and Frenkel defects. Thermodynamics of their formation, colour centers. Nonstoichiometric defects. Metal excess and metal deficiency defects. Line imperfections, edge dislocation and screw dislocation, Burger's circuits. Surface imperfection, `grain boundaries and stacking faults.

### Unit-III: Semiconductors and their devices

12 Hrs

Intrinsic and extrinsic semiconductors, semiconductors materials and their fabrication, semiconductors devices p-n junctions, properties of p-n junctions, semiconductors diode as rectifier, Filters circuits, Zener diode as a voltage stabilizer, transistors transistor as an amplifier Super conductivity: conventional super conductors, organic super conductors (organic metals), fullerece, high temperature super conductors, organic charge transfer complexes Applications.

### Unit-IV: Theories of solid state and properties of solids

12 Hrs

Free electron theory, Conduction by free electrons, Band theory, refinement to simple band theory, band structure of metals. Insulator and semiconductors. **Generation of x-rays, interaction of x-rays with matter, scattering and diffraction, Bragg's law, Miller indices, General instrumentation, Bragg's method, single crystal method, Debye-Scherrer method, Identification of unit cells from systematic absences, x-ray intensities and structure determination, structure factor and its relation to electron density and intensity, Phase problem. Indexing of lattice planes**

in a cubic system, structure of NaCl and KCl, Avogadro's number from cubic lattice dimensions, applications of x-ray diffraction.

### **Unit-V: Ceramics**

**12 Hrs**

Introduction, major component of ceramics, clays, silica, feldspar, clay minerals, classification of clay minerals, properties of clay minerals, pillared clays, principal of pillaring, variety of pillaring species, modification of pillared clays, preparation of pillared clays, catalytic applications.

### **Reference Books**

1. Solid State chemistry and its Applications-A. R. West (John Wiley and sons)
2. 2 Principles of Solid State –H.V. Keer (Wiley Eastern Limited)
3. Material science and Engineering-V.Raghavan (prentice Hall of India)
4. Principles of Electronics- V.K.Metha (S.Chand and co.)
5. Engineering chemistry –P.C. Jain and M. Jain (Shanpat Rai and Sons)
6. Industrial chemistry –B.K. Sharma (Goel publishing House)
7. Selected topics in solid state physics vol.12 The growth of crystals from liquids
8. J.C. Brice, North Hollond/American Elesvier(1973)
9. Chemistry of imperfect crystal-F.A. Krogen
10. Crystals and Crystal Growing, Alan Holden and Phylis Singer, Anchor Books Doubleday, New York, 1960
11. X-ray Structure Determination A Practical Guide, 2<sup>nd</sup> edition George H. Stout and Lyle H. Jensen, John Wiliey & Sons, New York, 1989.

## CHECP-303 :Thermodynamics

04 Hrs/Week

Credits: 04

Marks 100

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### Statistical Thermodynamics

#### Unit-I: Introduction

12hrs

Ensembles-canonical, grand canonical and micro canonical Combinatorial problems, Thermodynamics probability and most probable distribution, Stirlings approximation, distribution laws, the law of equipartition of energies. Quantum statistics- Max Well-Boltzmann, Bose-Einstein and Fermi-Dirac, limit and applicability of various distribution laws.

#### Unit-II: Molecular Partition function

12hrs

Partition function, Expression for translational, rotational, vibrational and electronic partition functions, Third law of thermodynamics and partition function, Numerical problems.

#### Unit-III: Application to chemical systems

12hrs

Partition function and Thermodynamic functions, Sackur-Tetrode equation (derivation), determination of equation of state of an ideal gas. Internal rotation, residual entropies, heat capacity of solids: Einstein model, Debye modification (model), characteristic temperature, statistical mechanics of solutions ideal and nonideal.

#### Unit-IV: Applications to quantum systems

12hrs

Nuclear spin statistics, ortho and para nuclear states, ortho and para hydrogen. Fermi energy, Fermi energy of electron gas in metals, Planck's distribution law and radiation, Bose-Einstein degenerate gas (He gas).

#### Unit-V: Irreversible Thermodynamics

12hrs

Postulates, entropy production in heat, entropy production in matter flow, entropy production in chemical reactions, Onsager's theory, microscopic reversibility and Onsager's reciprocity, stationary states and entropy production, Prigogine's principle of minimum entropy, application to thermoelectric effects-Seebeck and Peltier effect.



## Reference Books

- 1) Statistical Thermodynamics, Donald A. Mc Quirrie, Harper & Row, New York 1973.
- 2) Statistical Thermodynamics, M.C. Gupta, Wiley Eastern Ltd. New Delhi.
- 3) Elements of Statistical Thermodynamics, L. K. Nash Addison Wesley, Menlo Park, 1972.
- 4) Physical chemistry, P. W. Atkins, ELBS
- 5) Non Equilibrium Thermodynamics, Prologine Kalyani Publication.
- 6) Thermodynamics and Non Equilibrium Thermodynamics, Gurudeep & Raj.

## CHEEP-304 : Advanced electrochemistry

04 Hrs/Week

Credits: 04

Marks 100

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### Unit -I: Oxidation - Reduction Systems:

12 Hrs

Oxidation potentials, reversible ox-red systems, determination of standard ox-red potentials, variation of ox-red potential, ox-red equilibria, ox-red systems in analytical chemistry, ox-red indicators, two stage ox-red , semiquinone formation constant. Numericals.

### Unit-II: Bio- electrochemistry and Electrocatalysis

12 Hrs

Donnan membrane equilibrium, membrane potential, theories of membrane potential, introduction to electrocatalysis, relative power of electrocatalysts, mechanism of electrocatalysis, bioelectro catalysis, immobilization, application of enzymes on electrodes.

### Unit-III: Electrodeposition

12 Hrs

Introduction, the electrogrowth of metals on electrodes , the reaction pathway for electro deposition, surface diffusion of ions, cathodic deposition of metals from solutions, factors affecting cathodic deposition of metals, electrochemical dissolution and passivity of metals, anodic dissolution of metals, film and adsorption theories of passivity.

Electroplating of metals, mechanism, throwing power of an electroplating bath, factors affecting throwing power, typical electrodeposition processes, and applications of electroplating of metals. Numericals.

### Unit-IV: Polarization and Overpotentials

12 Hrs

Polarization, concentration polarization, decomposition potentials, over voltage, hydrogen, oxygen and metal overvoltages, types of overvoltages, factors affecting overvoltages, experimental determination of decomposition potential and overvoltage, Tafels theory and Tafel equation, simultaneous deposition of metals .Numericals .

### Unit-V: Conversion and storage of electrochemical energy

12 Hrs

Introduction of storage cells, fuel cells, solar cells Types of storage cells (batteries) ,measure of cell performance , charging and discharging , introduction of classical batteries , modern batteries –zinc-air , nickel-metal oxide and lithium batteries.

Brief history of fuel cells, efficiency of fuel cells, hydrogen-oxygen fuel cell, phosphoric acid fuel cell, direct methanol and biochemical fuel cells; Solar cells introduction, principle and working of solar cells, advantages.

**Reference Books :**

- 1) Modern Electrochemistry, Vol 1,2A and 2B, John O” M Bokris
- 2) An Introduction to Electrochemistry, Samuel Glasstone.
- 3) Theoretical Electrochemistry, L.Antropov.
- 4) Advanced Physical Chemistry, Gurtu and Gurtu.
- 5) Principles of Physical Chemistry, Puri,Sharma and Pathania.
- 6) Text Book of Physical Chemistry, S. Glasstone
- 7) Physical Chemistry, Robert J. Silbey.
- 8) Physical Chemistry, G.K.Vemulapalli.
- 9) Physical Chemistry, Maron and Pruton.
- 10) Physical Chemistry, P.W. Atkins

## CHEEP-305: Environmental chemistry

04 Hrs/Week

Credits: 04

Marks 100

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### Unit-I: Air Pollution

[12hrs]

General considerations: polluted air, Types of pollution and units of measurements. Air quality standards, Sampling, Monitoring, Analysis of CO, Sources and sinks of CO pollution, Effects of CO on plants and humans, Control of CO pollution, Analysis of oxides of nitrogen, NO<sub>x</sub> sources and sinks of NO<sub>x</sub> pollution, Control of NO<sub>x</sub> pollution, Hydrocarbons and photochemical smog and its control, Analysis of hydrocarbon in exhaust gasses, Petrol and air, Sulphur dioxide sources, Analysis and control, Acid rain particulates and their effects on human and climate, Control of particulates.

### Unit-II

[12 hrs]

**Water Pollution:** Aquatic environment, Water pollutants, Sampling of water and its preservation Trace metals in water, Chemical speciation with special reference to Copper, Lead, Mercury and Arsenic. Water quality standards Water quality parameters.

**Oxygen Demanding Wastes:** Dissolved oxygen, Biological oxygen demand, Monitoring techniques and methodology with special reference to ammonia, Nitrates, Nitrites, Fluorides, Cyanides, Total hardness, Lead, Cadmium and Mercury. Detection and control of Detergents, oils, Pesticides, Sewage treatment.

### Unit-III

[12 hrs]

**Chemical toxicology :** Toxic chemicals in environment, Impact of toxic chemicals on enzymes, Biochemical effects of Arsenic, Cadmium, Lead, Mercury, Carbon monoxide, Sulphur dioxide, Pesticides and Carcinogens.

**Soil analysis:** Sampling of soil, Determination of water holding capacity, Determination of total nitrogen, phosphorous and sulphur in soil.

### Unit-IV

[12hrs]

**Industrial pollution:** Pollution due to cement industry, Distillery, Pharmaceutical (Drug) industries, Sugar industry, Paper and pulp industries, Thermal power plants, Nuclear power plants, Metallurgical industries, Polymer industries. Recycle, reuse, recovery, disposal, and management of solid industrial waste.

## Unit-V: Pesticides and Environmental pollution

[12 hrs]

Types of pesticides, , Insecticides and Herbicides . Effect of pesticides, Insecticides and Herbicides on environment , Physicochemical decomposition of pesticides, , Insecticides and Herbicides by soil microorganism and other living organism .

### Reference Books

1. A. K. De, Environmental Chemistry, Wiley Eastern Ltd. New Delhi.
2. S. L. Chopra and J. S. Kanwar, Analytical, Agricultural Chemistry, Kalyani Publishers, New Delhi.
3. Environmental chemistry , V P Kudesia , Pragati prakashan , Meerut.
4. R. K. Trivedy and P. K. God, Chemical and biological methods for water pollution studies, Environmental publications, co. New Delhi.
5. L. A. Richards, Diagnosis and improvement of saline and alkali soils. Oxford IBH publications co. New Delhi.
6. S. M. Khopkar, Environmental chemistry, Environmental pollution analysis.
7. M. S. Creos and Morr, Environmental chemical analysis, American publications.
8. M. Sittig, Resources, Recovery and Recycling, Handbook of industrial waste.
9. Standard methods of water and waste water analysis, American public health association Washington D. C.
10. R. Gopalan and Amrutha Anand, "Environmental chemistry laboratory manual Emerald Publication.
11. Standards for water for drinking and other purposes, Bureau of Indian Standards India.
12. Guideline for drinking water quality recommendations of world health organization, Geneva.
13. B. K. Sharma and H. Kaur, Environmental Chemistry, Guel publishing house Meerut.
14. Thomas G. Spiro and William M. Stigliani, Chemistry of environment.
15. Green Chemistry: An Introductory Text, Mike Lancaster, Royal Society of chemistry(2002)
16. New Trends in green Chemistry, V.K. Ahluwalia and M. Kidwai, Anamaya Publishers New Delhi, (2004)

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## CHEEP:306 Nuclear chemistry

04 Hrs/Week

Credits: 04

Marks 100

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### Unit- I Nuclear particles and its properties

[12 hrs ]

The fundamental particles, roll call of elementary particles, composition of the nucleus, theories of nuclear composition, nuclear properties, mass defect and binding energy, nuclear stability explained by different factors.

Nuclear size and density, mechanical effects due to orbiting and spinning of nucleons, orbital angular momentum of the nucleons, Total angular momentum of the nucleons, magnetic quantum numbers, principal and radial quantum numbers, total angular momentum of nucleus, total magnetic nuclear angular momentum quantum number, magnetic properties of the nucleus, the neutron magnetic moment, the structure of nucleon the net magnetic moments, The spin of odd Z odd N nuclei, The Nordheim rule.

### Unit- II: Nuclear models

[12 hrs]

The shell model and its salient features, periodicity in nuclear properties- magic numbers, forces of nuclear potential, energy level in nuclear potential well, the sequence of filling the orbital including models, nuclear configuration. The liquid drop model, and its details and The Fermi gas model.

### Unit-III: Radioactivity

[12 hrs]

Historical, background, natural radioactive elements, general characteristics of  $\alpha$ ,  $\beta$ ,  $\gamma$  rays, detection and measurement of radioactivity, the theory of radioactive disintegration, decay kinetics, units of radioactivity, parent daughter growth relationship- secular and transient equilibrium, theory of  $\alpha$  decay,  $\beta$  decay – energetics of  $\beta$  decay problems of  $\beta$  decay, fermis theory of  $\beta$  decay, nuclear de-excitation – emission, numerical

### Unit-IV: Nuclear Reactions

[12 hrs]

Definition and Bethes notation, nuclear reaction energetic, nuclear reaction and threshold energy, characteristics of nuclear reactions, types of nuclear reactions, conservation in nuclear reactions, nuclear reactions cross section, cross section and reaction rate, the compound nucleus theory, general properties of compound nucleus, optical model, direct interaction model, specific nuclear

reactions- photonuclear reactions, stripping and pickup reactions evaporation, spallation, fragmentation, direct nuclear reactions, thermonuclear reactions.

#### **Unit-V: Radiation chemistry and its applications**

**[12 hrs]**

Introduction of radiation with matter, primary effects due to charged particle/radiation, Linear energy transfer(LET), Bethes equation for LET, Bremsstrahlung, the cerenkov radians, interactions of electron with matter, interaction of neutrons with matter, interaction of heavy charged particles with matter, interaction of rays with matter, units for measuring radiation absorption, absorption in water **B**. Typical reactions involved in the preparations of isotopes: the scillard-chalmers reactions, radiochemical principles in the use of tracers, typical application of radioisotopes as tracers- chemical investigation, physio-chemical research, analytical applications, agricultural applications, industrial applications, use of nuclear radiations, radioisotope as a source of electricity

#### **Reference Books.**

1. Source of Atomic energy by s. Glasstance, D. Van Nostrand co. INC
2. Essentials of nuclear chemistry by H.J. Arnikar 4<sup>th</sup> Edn, New Age International(p) Ltd.
3. Introduction to Nuclear By chemistry B. G. Harvey,
4. Nuclear chemistry by M. G. Arora & M. Singh Anmol publication, New Delhi
5. Elements of nuclear chemistry by A. K. Srivastav, P. C. Jain, S. Chand & Co.
6. A text book of Nuclear chemistry by C.V. Shekar Deminant publication & distribution, New Delhi.
7. Radiochemistry & nuclear chemistry, 3<sup>rd</sup> edn G. chappin, Butterwerth-Heinemann.

## CHELP-307 :Laboratory course

06 Hrs/Week

Credits: 03

Marks 50

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### Spectroscopy

- 1) To determine the indicator constant  $pK_{in}$  of an indicator by using half height method (Bromo cresol purple) (DVJ-200)
- 2) To determine the stability constant of metal complex between 5-SSA and  $Fe^{+3}$  with help of Job's curve and Bent and French method (for weak complex) (DVJ-204)
- 3) To determine the concentration of Fe(II) and Cu(II) by spectrophotometric titration with EDTA.
- 4) To investigate the reaction kinetics between  $K_2S_2O_8$  and KI by spectrophotometrically (TKC-223)
- 5) To determine simultaneously the dichromate and permagnate ions in the given solution.

### Polarimetry

- 6) Determine the percentage of two optically active substances in a mixture.(TKC-194)
- 7) To investigate the complex ion formation between Fe(II) and thiocyanate ion.
- 8) To study Kinetics of hydrolysis of sucrose by Hammett-Zuckerman approach.(DVJ)
- 9) Investigate the effect of substitution of chloride ions on rate constant of inversion of cane sugar by using mono, di and trichloro acetic acid as catalyst.

### Refractometry

- 10) Determine the refractive indices of series of solution of a salt and determine the concentration of the salt in the given unknown solution.
- 11) Study the variation of refractive indices with composition of mixture of carbon tetrachloride and ethyl acetate and determine the composition and molar refraction of the given unknown mixture.



## **Viscosity**

- 12) Determine the variation of viscosity with composition of I) ethanol-water, II) methanol-ethylidene chloride, III) nitric acid- chloroform and and conform the formation of compound.(TKC-250)
- 13) Determine the molecular weight of macromolecules.(TKC-251)
- 14) Determine the iso-electric point of gelatin and examine the effect of aging by viscometric methods.(DVJ-29)

## **Flame Photometry**

- 15) Estimation of Na, K, Li & Ca by flame photometry.

### **Reference Book**

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

## CHELP- 308 : Laboratory course

06 Hrs/Week

Credits: 03

Marks 50

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### Potentiometer

- 1) Titrate ferrous ammonium sulphate with ceric sulphate and find out formal redox potential of  $\text{Fe}^{+2}/\text{Fe}^{+3}$  and  $\text{Ce}^{+3}/\text{Ce}^{+4}$  system
- 2) Titrate potentiometrically phosphoric acid solution against NaOH and calculate  $\text{pK}_1$ ,  $\text{pK}_2$  and  $\text{pK}_3$  of the acid.
- 3) To determine the standard free energy changes  $\Delta G^\circ$  and equilibrium constant for reaction  $\text{Cu} + 2\text{Ag}^+ \longrightarrow \text{Cu}^{++} + 2\text{Ag}$  (TKC-167)
- 4) Determine the activity coefficient of silver ions using a concentration cell without transference.(TKC-154)

### pH metry

- 5) To determine the proton-ligand stability constant of an organic acid and the metal-ligand stability constant of its complex by pH measurements.(TKC-176)
- 6) Determine the Hammett constant of a given substituted benzoic acid by pH measurements.(TKC-170)
- 7) Determine the pH values of various mixtures of sodium acetate and acetic acid in aqueous solution and hence find out the dissociation constant of the acid.(TKC-173)
- 8) To determine the hydrolysis constant of aniline hydrochloride by pH measurements. (TKC-174)

### Conductometry

- 9) Conductometric titration of a mixture of strong acid, weak acid and a salt.(DVJ )
- 10) To determine the degree of hydrolysis and hydrolysis constant of sodium acetate conductometrically.
- 11) Determine the amount of trichloroacetic acid, monoacetic acid and acetic acid in a given solution by conductometric titration against sodium hydroxide solution.

### **Magnetochemistry**

- 12) To determine the magnetic susceptibility and number of unpaired electrons in given compound.
- 13) Verification of Weidemann's law using nickel chloride solution.

### **Surface Tension**

- 14) Study the effect of surfactant (n-propyl alcohol) at various concentrations on the surface tension of water and hence determine the limiting cross sectional area of alcohol molecule by stalagmometer.
- 15) To study the effect of surfactant on surface tension of water by parachor of a solid by stalagmometer.

### **Reference Book**

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

## CHELP-309 : Laboratory course

06 Hrs/Week

Credits: 03

Marks 50

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### Chemical Dynamics

- 1) Investigate the influence of ionic strength on the rate constant of the reaction between  $K_2S_2O_8$  and KI.(TKC-335)
- 2) Determine the order of a reaction by 1) substitution method, (II) fractional change method and (III) differential method.
- 3) Investigate the reaction between bromic acid and hydrochloric acid.(TKC-335)
- 4) Investigate the kinetics of iodination of acetone.

### Phase equilibria

- 5) Determine the critical solution temperature of phenol and water in presence of 1) 1% NaCl 2) 0.5% naphthalene 3) succinic acid
- 6) Construct the phase diagram of three-component system containing ethanol benzene and water.
- 7) Determine the equilibrium constant of the tri-iodide formation in aqueous solution by distribution method.
- 8) Determine the formula of the complex formed between cupric ion and ammonia by distribution method.

### Adsorption

- 9) Investigate the adsorption of acetic / oxalic acid by activated charcoal and test the validity of Freundlich and Langmuir's isotherm.

### Thermodynamics

- 10) Determine the partial molar volume of ethanol and water in a given composition by density measurements.
- 11) To determine heat of neutralization of strong acid and heat of ionization of weak acid calorimetrically.
- 12) To determine the integral heat of solution of  $KNO_3$ .

13) To determine the heat of dissociation of benzoic acid in water.

14) To determine heat of precipitation of  $\text{BaSO}_4$ .

### **Turbidimetry**

15) Determine the molecular weight of a given polymer by turbidimetry

### **Reference Book**

1. Systematic experimental physical chemistry – T. K. Chondhekar & S.W. Rajbhoj

2., Experiments in chemistry – D.V. Jahagirdar

## CHECP-401: Surface and magnetochemistry

02 Hrs/Week

Credits: 02

Marks 50

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### Unit-1: Surface Chemistry

[10 hrs]

Adsorption, adsorption isotherms, Langmuir's unimolecular theory of adsorption statistical derivation of Langmuir's adsorption isotherm, BET theory of multilayer adsorption and its determination

### Unit-2: Colloidal state of Matter

[10 hrs]

Introduction to colloids, classification, properties, specific properties like, electrical properties, charge on colloidal particles, origin of charge, electrical double layer, electrokinetic properties, electrophoresis, electroosmosis, streaming potential, sedimentation potential, determination of size of colloidal particles, applications of colloids, Numericals.

### Unit-3: Introduction to Magnetochemistry

[10 hrs]

Definition of magnetic properties, types of magnetic behaviour, sources of paramagnetism, Pascals constants and its applications, Determination of magnetic susceptibility. Numericals.

### Reference Book

1. K.J.Laidler, J.H.Meiser and B.C. Sanctuary, Physical Chemistry, Houghton Mifflin Company, New York, 2003.
2. A.W. Adamson, Physical Chemistry of Surfaces, 4 th edition, Interscience, New York, 1982.
3. G.K.Vemulapalli, Physical Chemistry, Printice Hall of India.
4. Gurtu and Gurtu , Advanced Physical Chemistry.
5. S.Glasstone, Text book of Physical Chemistry.
6. Gurdeep and Raj, Advanced Physical Chemistry.
7. A.R.West, Solid State Chemistry and its Applications, John Wiley and Sons, 2003(reprint 2009)
8. H.V.Keer, Principles of Solid State.
9. A.Earn Shaw, Introduction to Magnetochemistry, Academic Press.
10. J.Sharma, Magnetochemistry.
11. R.I.Dutta and Syamal, Elements of magnetochemistry.

## CHECP-402 : Polymer chemistry

04 Hrs/Week

Credits: 04

Marks 100

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### Unit-I: Fundamentals of Biological Macromolecules

[12 hrs]

Chemical bonds in biological systems; Properties of water; Thermodynamic principles in biological systems; Properties and classification of amino acids; Structures of nucleic acids, Protein structure and function, Properties of nucleosides and nucleotides, Composition of nucleic acids, Electrophoresis, Factors affecting on Electrophoretic Mobility; Types of Electrophoresis; Free electrophoresis and Gel electrophoresis; Electrophoresis in genetic analysis; DNA Sequencing and DNA foot Printing.

### Unit-II: Macromolecules

[12 hrs]

Introduction, Formation of synthetic high polymers classification, Polymerization reactions: Chain and Step. Average molecular weight, Number average weight, Methods of determination of molar masses of polymers; Viscosity, Osmometry, Molar mass of charged macromolecules, Donnan membrane equilibrium, Ultracentrifugation, light scattering, Diffusion.

### Unit-III: Chemistry of Polymerization

[12 hrs]

Chain polymerization: free radical polymerization, ionic polymerization, co-ordination polymerization, Ziegler-Natta catalysts. Step Polymerization: polycondensation, polyaddition, ring opening, electro chemical polymerization, group, Transfer polymerization, Polymerization techniques.

### Unit-IV: Kinetics of Polymerization

[12 hrs]

Free radical chain polymerization, Anionic polymerization, Cationic polymerization, Copolymerization, Free radical copolymerization, Ionic copolymerization, Copolycondensation.

### Unit-V: Electronically Conducting Polymers

[12 hrs]

Introduction, Theories of electronic conduction; Band theory of conduction, Hopping conduction, Super conduction, Mechanism of conduction, Doping mechanism, p-type, n-type, auto doping, Stimuli sensitive (smart) polymers, pH and temperature sensitive smart polymers, Applications: Photovoltaic devices, Sensors, LED and Solar cells, Electro chemical devices, Batteries etc.

## Reference Book

1. Cantor, C. R. and Schimmel Biophysical Chemistry Vols. 1-3, W. H. Freeman (1980).
2. Lehninger, A.L., Nelson, D. L. and M. M. Lehninger, Principles of Biochemistry 4<sup>th</sup> Ed., W. H. Freeman (2004).
3. U. Satyanarayana; Biochemistry.
4. Upadhyay; Biophysical Chemistry.
5. L. Stryer, Biochemistry, 5<sup>th</sup> Edition, (2002) Freeman and Co. New York.
6. D. Voet, J. G. Voet, Biochemistry 3<sup>rd</sup> Edition (2004), Wiley International Publication.
7. D. L. Nelson and M. M. Cox, Lehninger Principles of Biochemistry 3<sup>rd</sup> Edition (2002) McMillan North Publication.
8. Polymer Science. By V. R. Gowariker, N. V. Viswnathan, Jayadev Sreedhar.
9. Polymers and Resins. By Brage Golding.
10. Electrical Properties of Polymers. By Tony Blythe and David Bloor.
11. Self doped conducting polymers. By Michael S. Freund and Bhavana Deore.
12. Polymer Science and Technology. By Premamoy Ghosh.



## CHECP-403: Chemical dynamics and catalysis

04 Hrs/Week

Credits: 04

Marks 100

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### Unit-I: Kinetics of Complex Reactions

[12 hrs]

Opposing or reversible reactions, parallel and competitive reactions, consecutive reactions, chain reactions, branched chain reactions and explosions, hydrogen-oxygen reactions, kinetics of polymerization-step wise and free radical polymerization Effect of temperature on rates of simple and complex reactions. Numericals

### Unit-II: Reactions in solution

[12 hrs]

Diffusion controlled reactions, substitution and correlation effect, Hammett equation, Taft effects, compensation effect. Electron transfer reactions, proton transfer reactions. Ion dipole and dipole-dipole interactions. Influence of pressure on rate in solution. Numericals

### Unit-III: Photochemical Reactions

[12 hrs]

Introduction, law of photochemical equivalence, photocatalytic reactions, types of photocatalytic reactions, photooxidation, photoreduction, photosensitization, photocatalytic degradation. Chemiluminescence, photosynthesis. Numericals

### Unit-IV: Homogeneous Catalysis

[12 hrs]

Introduction, mechanism of catalysis, Acid-base catalysis, effect of pH on rate constant. Micellar catalysis, enzyme catalysis, factors governing rate of enzyme reactions, kinetics of enzyme catalysed reactions. Autocatalysis and oscillatory reaction, Lotka-Volterra mechanism, the Brusselator, the Oregonator, bistability, chemical chaos. Numericals

### Unit-V: Surface reactions and Heterogeneous catalysis

[12 hrs]

Unimolecular surface reactions, bimolecular surface reactions, effect of temperature on heterogeneous reactions, transition state theory and the rates of surface reactions, theory of heterogeneous catalysis, structure of solid surfaces, absolute rates of desorption's, electronic theories of chemisorption and heterogeneous catalysis. Preparation and characterization of catalysts, applications.

### Reference Books

1. Chemical kinetics- E.S.Laidler Pearson Education

Chemical kinetics and Reaction dynamics -Bul Houston

Chemical kinetics and Reaction Mechanism -F-Wilkinson-VanNostral Reinhdd

2. kinetics and Mechanism Of Chemical TransformationsJ. Rajaram Macmillan India Ltd  
J.C.Curiacose.
3. Physical chemistry- Atkin and D.Paula, Oxford University press
4. Physical chemistry- Berry, Rice, Ross Oxford University press
5. Physical chemistry-principles And Appllication in Biological Sciences -Tinoco, Sauer  
Pearson Education.
6. Physical chemistry-W.J.Moore.

## CHECP-404: Nanochemistry

04 Hrs/Week

Credits: 04

Marks 100

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### **Unit-I: General introduction & synthesis of nanomaterials by physical methods [12Hrs]**

Objective of study, synthesis of nanoparticles by physical method, mechanical methods- high energy ball milling, melt mixing, method based on evaporation, physical vapour deposition with consolidation. Ionized cluster beam deposition. Laser vaporization, Laser pyrolysis, sputter deposition, electric arc deposition, Chemical Vapour Deposition (CVD).

### **Unit-II: Synthesis of Nanomaterials by Chemical Methods [12Hrs]**

Introduction, colloids and colloids in solution, interaction of colloids and medium, colloids in vacuum, colloids in medium, effect of charge on colloids, steric repulsion, synthesis of colloids, growth of nanoparticles, synthesis of metal and semiconductor nanoparticles by colloidal route, Langmuir-Blodgett (L-B) method, sol gel method, electrochemical method.

### **Unit-III: Analysis Technique [12Hrs]**

Introduction, microscopes, electron microscopes, SEM, TEM, Scanning probe microscope (SPM), Scanning Tunnelling microscope, Atomic force microscope, X-ray diffraction, UV-visible and IR spectroscopy.

### **Unit-IV: Properties, types and application of Nanomaterials [12Hrs]**

Properties of nanomaterials – Mechanical, electrical, optical, magnetic, semiconductor.

- i. *Some special nanomaterials – Carbon nanotubes, porous silicon, Arogels, Zeolites.*
- ii. *Application – Electronic, energy automobiles, sport and toys, textile, cosmetics, domestic appliances, biotechnology, medical, space, defence & environment.*

### **Unit-V: Thin films: [12Hrs]**

Introduction, deposition by chemical reactions, deposition by electrochemical reaction, chemical vapor deposition of inorganic Thin films, chemical etching.

### **Reference Books:**

1. Nanotechnology: Principles and practices- Sulabha K. Kulkarni (capital Pub. Co.)
2. NANO- The next revolution –Mohan Surendra Rajan(Natioinal book Trust, India)
3. The British Glass Website- Types of Glass://www.britiglass.org.uk.

4. Fundamental of Nanotechnology – Gabor L. Hornyak, John J. Moore, Harry F. Tibbals, Joydeep Dutta.
5. Recent advances in the liquid phase synthesis of Inorganic Nanoparticles- B. LCushing, V. L. Kolesmichenko & C.J.O”.Connor Chemical Review 104, 3893-3946.(2004)
6. Hand book of Thin film technology- H. R. Khan.
7. Thin film phenomenon- K. N. Chopra. Mcgrawa Hill publication
8. Material Science deposition & structure –Milton.

## CHECP -405: Instrumental methods of chemical analysis

04 Hrs/Week

Credits: 04

Marks 100

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### Unit-I: General Introduction

[12hrs]

Overview of Electrode Processes, Electrocapillary curve and electrocapillary maximum potential, exchange current, Ion selective electrodes: Types and construction of electrode, Glass electrode, Solid state electrode and precipitate electrode, Liquid-liquid membrane electrodes, Enzyme and gas electrode, Applications of ion selective electrodes, Reference electrodes, Mercury electrodes (DME, SME, HMDE), numericals.

### Unit – II: Potentiometry and Coulometry

[12hrs]

**Potentiometry:** Introduction, Instrumentation, Various electrodes in potentiometry:- Ion selective electrode, Liquid membrane electrode, Weston cell. Potentiometric titrations:- Types of potentiometric titrations, Variations in potentiometric titrations, Limitations, Numericals.

**Coulometry:** Introduction, Principle, Technique, Coulometry at constant current and coulometry at controlled potential, Coulometric titration, Flowing stream coulometry, Applications, Stripping analysis.

### Unit- III: Cyclic Voltammetry

[12hrs ]

Theory and origin of polarography, Interpretation of polarographic curves, Instrumentation of polarography, Differential pulse polarography, Factors affecting on polarographic wave. Introduction and beginning of cyclic voltammetry Range of cyclic voltammetric techniques, Limitations. The acceptable sweep rate range, The shape of the peak in potential sweep curves, The role of non- aqueous solution in cyclic voltammetry, Criteria of reversibility of electrochemical reactions Quasi reversible and irreversible processes, Qualitative and quantitative analysis by cyclic voltammetric techniques, Linear sweep voltammetry for reactions that include simple adsorbed intermediates and Numericals.

### Unit-IV: Molecular Luminescence Spectrometry

[12hrs]

Theory of fluorescence and phosphorescence, Instruments for measuring fluorescence and phosphorescence, Applications and photoluminescence methods, Chemiluminescence.

### Unit – V: Thermal methods of analysis

[12 hrs]

General introduction, classification of thermal methods of analysis thermogravimetry, principles, factors affecting thermal curve, thermogravimetric analysis, Derivative thermogravimetry, Differential thermal analysis - principles, factors affecting DTA curve, applications, differential scanning calorimetry - principles, instrumentation and applications, thermomechanical and dynamic mechanical analysis, thermometric titrations, numericals.

**Reference Books:**

1. Quantitative analysis -. Alexeyev. V
2. Instrumental methods of analysis – Chatwal and Anand.
3. Introduction to instrumental analysis – R. D. Braun.
4. Instrumental methods of analysis – Willard, Meritt, Dean and Settle.
5. Standard methods of chemical analysis – F. G. Welcher, Vol III, Part A& B.
6. Electroanalytical chemistry – H. W. Neurenberg.
7. Principles of electrochemistry – D. A. MacLines.
8. Ion selective electrodes – (John Wiley) Stulic.
9. Vogel's textbook of quantitative chemical analysis V edition by Jeffery Bassett Mendham Denney.
10. Modern Electrochemistry vol. I - John O'M Bockris
11. Modern Electrochemistry vol. II - John O'M Bockris
12. Analytical Chemistry – Gary D. Christian, 6<sup>th</sup> edition
13. Principles of Instrumental Analysis–Skoog, F. J. Holler & J. A. Nieman.
14. Instrumental Methods of Chemical Analysis–Galen W. Ewing. 5<sup>th</sup> edition

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## CHECP- 406 : Biophysical chemistry

04 Hrs/Week

Credits: 04

Marks 100

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### Unit-I: Biomolecules and Bioenergetics

[12 hrs]

Biomolecules and the cells, carbohydrates, lipids, proteins and amino acids, nucleic acids and nucleotides, enzymes and vitamins, Free energy change in biochemical reactions, exergonic, endergonic, hydrolysis, ATP Biological oxidation reaction

### Unit-II: Centrifugation

[12 hrs]

Basic principle of centrifugation, Instrumentation, desktop centrifuges, high speed centrifuge, the ultracentrifuge, analytical centrifuges, rotors, differential, density gradient, analytical centrifugation.

### Unit-III: Electrophoresis

[12 hrs]

Factors affecting electrophoretic mobility, types of electrophoresis, free electrophoresis, zone electrophoresis and gel electrophoresis, electrophoresis in genetic analysis, DNA sequencing and DNA foot printing.

### Unit-IV: Isotopes in biology

[12 hrs]

Radioactive decay, production of isotopes, interaction of radioactivity with matter, measurement of radioactivity, gas ionization methods, photographic method and excitation method, use of stable isotopes in biology, the tracer techniques, use of isotopes as tracer, commonly used isotopes safety aspects.

### Unit-IV: Bio- statistical Analysis

[12 hrs]

Frequency distribution, T- test, Chi- square test, analysis of variance, co-relation and regression.

### Reference Books:

1. U. Satyanarayana; Biochemistry.
2. Upadhyay; Biophysical Chemistry.
3. L. Stryer, Biochemistry, 5<sup>th</sup> Edition, (2002) Freeman and Co. New York.
4. Lehninger, A.L., Nelson, D. L. and M. M. Lehninger, Principles of Biochemistry 4<sup>th</sup> Ed., W. H. Freeman (2004).
5. Biophysical Chemistry.- M. Satake
6. Biostatistical Analysis- A. M. Mungikar

**CHEPR-407 : Research project (Experimental)**

**24 Hrs/Week**

**Credit : 12**

**200 Marks**

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**CHEPR-408 :Research project (Dissertation, presentation and Seminars)**

**6 Hrs/week**

**Credit : 6**

**100 Marks**

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**DR. BABASAHEB AMBEDKAR MARATHWADA UNIVERSITY,**

**AURANGABAD**

**DEPARTMENT OF CHEMISTRY**

**Revised Syllabus**

**M. Sc. III & IV Semester Analytical Chemistry**

**Effective from June 2017**

The following will be the Choice Based Credit and Grading System structure of revised syllabus for M. Sc. III & IV semester Analytical Chemistry effective from June 2017.

Semester	Paper Nos.	Title of Paper	Teaching (Hrs.)/week	Marks	Credits
III- Semester	CHESC-301	Structural elucidation by spectral methods	04	100	04
	CHECA- 302	Advanced Analytical Techniques-I	04	100	04
	CHECA- 303	Quality Assurance and Accreditation	04	100	04
	CHEEA -304	Electroanalytical Techniques <b>OR</b>	04	100	04
	CHEEA -305	Advanced Analytical Techniques-II <b>OR</b>	04	100	04
	CHEEA- 306	Polymer & Petrochemical Analysis	04	100	04
	CHELA- 307	Laboratory course	06	50	03
	CHELA- 308	Laboratory course	06	50	03
	CHELA- 309	Laboratory course	06	50	03
IV semester	CHECA -401	Analytical Method Development and Validation	02	50	02
	CHECA -402	Pharmaceutical, and Forensic Analysis	04	100	04
	CHECA -403	Environmental Analysis and Monitoring	04	100	04
	CHEEA -404	Food, Fertilizer & Pesticides Analysis <b>OR</b>	04	100	04
	CHEEA -405	Ores, Alloys & Cosmetics Analysis <b>OR</b>	04	100	04
	CHEEA -406	Microbial and Clinical Analysis	04	100	04
	CHEAR - 407	Research project (Experimental)	24	200	12
	CHEAR - 408	Research project (Dissertation, Presentation and Seminars)	06	100	06

**UNIT-I Nuclear Magnetic Resonance Spectroscopy ( $^1\text{H}$  NMR) [12 hrs ]**

Elementary ideas (Recapitulation); Spin-spin couplings, Different types of couplings, factors affecting on coupling constants, Karplus equation, Spin systems (AB, AX, ABX, AMX), Rate processes, spin decoupling, shift reagents, Nuclear Overhauser effect (NOE), INEPT and INADEQUATE.

**UNIT-II  $^{13}\text{C}$  Nuclear Magnetic Resonance Spectroscopy [12 hrs ]**

Elementary ideas, instrumental problems, chemical shifts (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbons); Effect of substituents on chemical shifts.

**UNIT-III Mass Spectroscopy [12hrs]**

Introduction, ion production (EI, CI, FD and FAB), ion analysis, ion abundance, factors affecting on fragmentation, fragmentation of different functional groups, molecular ion peak, isotopic peaks, metastable peak, Nitrogen rule, McLafferty rearrangement, Retro-Diels-Alder reaction.

**UNIT-IV [12 hrs]**

Problems based on joint applications of UV, IR,  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and Mass spectroscopy.

**UNIT-V [12 hrs ]**

**(A) Mossbauer spectroscopy:** Principle, factors affecting the line position and shape, isomer effect and Quadrupole splitting iron salt like compounds, complexes, carbonyl compounds (temperature dependence of isomer shift and Quadrupole splitting in simple compound and coordination, polynuclear complexes), Numericals.

**(B) Electron Spin Resonance Spectroscopy:** Introduction, principle of ESR spectroscopy, presentation of spectrum, hyperfine splitting in various structures, hyperfine splitting diagram of representative examples, factors affecting the magnitude of 'g' values, Zero field splitting, Kramer's degeneracy, Anisotropy in the hyperfine coupling constant, electron delocalization, instrumentation and applications.

**Reference Books:**

1. Introduction to Spectroscopy: D. L. Pavia, G. M. Lampman, G. S. Kriz
2. Spectrometric Identification of Organic Compounds: R. M. Silverstein & F. X. Webster
3.  $^{13}\text{C}$  NMR Spectroscopy: G. C. Levy, R. L. Lichter, G. L. Nelson
4. Spectroscopic Methods in Organic Chemistry: D. H. Williams & I. Fleming
5. Absorption Spectroscopy of Organic Compounds: V. M. Parikh
6. Mass Spectrometry: K. G. Das & James
7. Coordination Chemistry by Experimental Methods: K. Barger
8. Coordination Chemistry vol. I: E. Martell
9. Physical Methods for Chemistry: R. S. Drago
10. Structural Methods in Inorganic Chemistry: E. A. V. Ebsworth & D. W. H. Rankin
11. Organic Structure Analysis: Philips Crews

**Unit-I. Chromatographic Systems**

**12 hrs.**

**Thin layer Chromatography:** Introduction, principles, superiority of tlc over other chromatographic technique, experimental techniques, solvent systems, plate development, detection of components, evaluation of chromatogram by different methods, applications, limitation. High performance thin layer chromatography

**Liquid-Liquid partition chromatography:** Introduction, theory, solid supports, selection of stationary and mobile phases, solvent systems, reverse phase chromatography, choice of adsorption or partition, applications of partition chromatography. Ultra performance liquid chromatography

**Column Chromatography:** Principle, experimental details, theory of development, column efficiency, factors affecting column efficiency, and applications. Advanced flash chromatography

**Gel permeation Chromatography:** Principle materials, gel preparation, column packing, detectors and applications.

**Ion Exchange Chromatography:**

Ion Exchange resins, ion exchange equilibria, ion exchange capacity of resins and its determination, applications of ion exchange resins to chromatography, ion chromatography based on suppressors

**Unit-II Gas Chromatography:**

**12hrs**

Introduction, principles of gas-liquid chromatography, instrumentation - Carrier gas, sample

Introduction system, columns, detectors, substrates, temperature control, evaluation

Retention volume, resolution, branches of gas chromatography, applications, numericals.

**High Performance Liquid Chromatography:**

Principle, instrumentation - column, column packing, mobile phase, pumping system, detector system, practical procedure, applications, HPLC adsorption and partition chromatography.

**Unit-III**

**12 hrs.**

Properties of Supercritical Fluids, Supercritical Fluid Chromatography, Supercritical Fluid Extraction.

Introduction, Need for hyphenation, Possible hyphenation, Interfacing devices and applications of the following: LC-MS, GC-IR, GC-MS, ICP-MS, MS-MS.

**Unit-IV Molecular Luminescence Spectrometry:** **12 hrs.**

Theory of fluorescence and phosphorescence, Instruments for measuring fluorescence and phosphorescence, Applications of photoluminescence methods, Chemiluminescence

**Unit-V Surface Characterization by Spectroscopy and Microscopy:**

**12 hrs.**

Introduction to the study of surfaces, Spectroscopic surface methods, Ion spectroscopic techniques, Surface photons spectroscopic methods, Electron stimulated microanalysis methods, Scanning probe microscopes

**Reference Books**

1. Instrumental Methods of Analysis–Willard, Merritt, Dean & Settle.
2. Instrumental Analysis- Skoog, Holler, Crouch.6<sup>th</sup> edition
3. Principles of Instrumental Analysis–Skoog, F.J.Holler & J.A.Nieman
4. Instrumental Methods of Chemical Analysis–Galen W. Ewing.
5. Analytical Chemistry – Gary D. Christian, 6<sup>th</sup> edition
6. Handbook of Instrumental Techniques for Analytical Chemistry –Frank Settle,Editor
7. Introduction to Instrumental Analysis-R.D. Braun, McGraw Hill.
8. Fundamental of Analytical Chemistry,-D.A. Skoog, D.M.West and F.J. Holler.
9. Wilson and Wilson Compressive Analytical Chemistry. Ed. G. Svehla, A series of volumes.
10. Instrumental methods of analysis – Chatwal and Anand.
11. Instrumental methods of analysis – B. K. Sharma.

**Quality Assurance and Accreditation****Unit-I Quality Assurance****15 hrs.**

**Introduction to Quality Control and quality assurance:** Concepts and significance. Quality control and statistical techniques: Quality control charts, the X-quality control chart, the R-quality control chart and its interpretation, spiked sample control charts, use of blind samples in quality control, use of proficiency evaluations in quality control.

**Calibration and maintenance of Instruments / Equipment:** Instrument calibration – linear calibration curves, equipment calibration, frequency of calibration, calibration of common laboratory instrument and equipment (Analytical balances, volumetric glassware, ovens, furnaces, UV / Visible spectrophotometer, pH meter, conductivity meter, IR spectrophotometers, AAS, GC, HPLC etc.). Maintenance of instruments and equipment

**Unit-II Documentation for quality assurance: Raw Data –****15 hrs**

Type of notebooks, control of notebook distribution and data entry. General Reagents and volumetric reagents. Sampling – sampling methods, sample labelling, sample log-in/register. Sample analysis, reporting, recording and personal training. Instrument calibration and maintenance. Analytical report. Personnel, training, records - professional personnel, technician personnel. Filing quality assurance documentation.

**Good laboratory practices** and personnel, Quality Programme, Instrument and Organisation calibration, Customer Satisfaction.

**Unit-III Documentation for quality assurance: Raw Data –****15 hrs**

**Computers and quality assurance:** Sample handling. Data Acquisition. Quality control data and calculations. Computer generated analytical reports. Security considerations. Hardware and software.

**Establishing a Quality Assurance program:** Management commitment. Define the quality assurance program. Writing standard operating procedures. Topics for standard operating procedures. Consolidating the programme. Monitoring the program – monitoring quality assurance data, reporting quality assurance problems. Writing the quality assurance manuals. AC( CB1) -4: Quality Accreditation:

**Unit-IV Quality Accreditation:****15 Hrs**

**Laboratory Accreditation:** Need for laboratory accreditation. International aspects of laboratory accreditation and in India. Criteria for laboratory accreditation. Benefits of laboratory accreditation, Evolution and significance of Quality Management, Background to ISO 9000, comparison between ISO-9001, ISO-9002 & ISO-9003., ISO 9000-2000 series of standards on quality management system, - evolution of series of standards, introduction to ISO organization, Registration / certification - benefits of QMS certification. Structure of ISO 9000-2000 family of standards. Advantages of ISO 9000-2000. Requirements of ISO 9001-2000 QMS and applications, Steps for effective implementations. Significance of ISO - 9001,9002,9003 & 9004. Requirements of ISO9000/IS14001. Concepts of OHSMS (BS 8800) Quality Management Principles in QMS, QMS documentation, Quality Manual, Quality policy, conformities and Non-conformities

**Reference Books:**

1. Handbook of Quality Assurance for the analytical chemistry laboratory, James P. Dux, Van Nostrand Reinhold, New York, 1986.
2. Applying ISO-9000 Quality Management Systems, International Trade Centre Publishing, UNCTAD/WTO. Geneva, Switzerland, Indian Edition Printed by D.L.Shah Trust.
3. How to practice GLP, PP Sharma, Vandana Publications, 2000, New Delhi
4. Training manuals on ISO 9000 / 2000 PQM, Girdhar J Gyani, Raj Publishing House, 2001
5. Quality Assurance in Analytical Chemistry, B.W. Wenclawiak, Springer,India, 2004.

**Unit-I General Introduction and Potentiometry [12 hrs ]**

Overview of Electrode Processes, Electrocapillary curve and electrocapillary maximum potential, exchange current, Ion selective electrodes: Types and construction of electrode, Glass electrode, Solid state electrode and precipitate electrode, Liquid-liquid membrane electrodes, Enzyme and gas electrode, Applications of ion selective electrodes, Reference electrodes, Mercury electrodes (DME, SME, HMDE), Numericals.

**Potentiometry:** Introduction, Instrumentation, Potentiometric titrations:- Types of potentiometric titrations, Variations in potentiometric titrations, Limitations, Numericals.

**Unit – II Coulometry and High frequency titration [12 hrs ]**

**Coulometry:** Introduction, Principle, Technique, Coulometry at constant current and coulometry at controlled potential, Coulometric titration, Flowing stream coulometry,,Stripping analysis,Applications

**High frequency titration** Introduction, Theory and instrumentation, High frequency titrimetry, Types of cells, Advantages of high frequency methods,Applications.

**Unit- III Polarography and Cyclic Voltammetry [12hrs]**

Theory and origin of polarography, Interpretation of polarographic curves, Instrumentation of polarography, Differential pulse polarography, Factors affecting on polarographic wave.

Introduction and beginning of cyclic voltammetry, Range of cyclic voltammetric techniques. The acceptable sweep rate range, The shape of the peak in potential sweep curves, The role of non-aqueous solution in cyclic voltammetry, Criteria of reversibility of electrochemical reactions, Quasi reversible and irreversible processes, Qualitative and quantitative analysis by cyclic voltammetric techniques, Linear sweep voltammetry for reactions that include simple adsorbed intermediates, Amperometric titrations, Chronoamperometry, Chronopotentiometry and others Numericals.

**Unit-IV [12 hrs ]**

**Electro-Gravimetry:** Introduction, Theory of electrogravimetry, Instrumentation,Electrogravimetric determination with constant applied voltage and constant current, Applications of electrogravimetry, Problems based on effect concentration on electrode potential, Calculation of theoretical potential, Effect of pH in electrolytic separation, Numericals

**Unit-V [12 hrs ]**

**Electrophoresis:** Introduction, Paper electrophoresis Principle, Experimental techniques, Factors governing migration of ions, and Applications, Numericals.

**Capillary and zone electrophoresis:** Electroosmotic flow, Migration in CE, Instrumentation, Control of separation, Application.

Gel electrophoresis: Principle,technique, application.

**Reference Books:**

1. Quantitative analysis -. Alexeyev. V
2. Instrumental methods of analysis – Chatwal and Anand.
3. Introduction to instrumental analysis – R. D. Braun.
4. Instrumental methods of analysis – Willard, Meritt, Dean and Settle.
5. Standard methods of chemical analysis – F. G. Welcher, Vol III, Part A & B.
6. Electroanalytical chemistry – H. W. Neurenberg.
7. Principles of electrochemistry – D. A. MacLlines.
8. Ion selective electrodes – (John Wiley) Stulic.
9. Vogel's textbook of quantitative chemical analysis - Mendham, Denney,etc.
10. Modern Electrochemistry vol. I - John O'M Bockris
11. Modern Electrochemistry vol. II - John O'M Bockris
12. Analytical Chemistry – Gary D. Christian, 6<sup>th</sup> edition
13. Principles of Instrumental Analysis–Skoog, F. J. Holler & J. A. Nieman.
14. Instrumental Methods of Chemical Analysis–Galen W. Ewing. 5<sup>th</sup> edition

**Unit-I Atomic Mass Spectrometry****12 hrs**

Some general features of atomic mass spectrometry, Mass spectrometers, Inductive coupled plasma mass spectrometry Spark source mass spectrometry, Glow discharge mass spectrometry, Other mass spectrometric methods.

**Unit-II Atomic X-ray Spectrometry****12 hrs**

Fundamental principles, Instrument components, X-ray fluorescence methods, X-ray absorption methods, The electron microprobe.

**Unit-III Thermal Methods****12 hrs**

General introduction, classification of thermal methods of analysis thermogravimetry, principles, factors affecting thermal curve, thermogravimetric analysis, Derivative thermogravimetry, Differential thermal analysis - principles, factors affecting DTA curve, applications, differential scanning calorimetry - principles, instrumentation and applications, thermomechanical and dynamic mechanical analysis, thermometric titrations, numericals. Microthermal analysis.

**Unit-IV Diffraction Methods:****12 hrs**

Generation of x-rays, interaction of x-rays with matter, scattering and diffraction, Bragg's law, Miller indices, General instrumentation, Laue Photograph method, Bragg's method, their principle and uses, single crystal method, Debye-Scherrer method, Identification of unit cells from systematic absences, x-ray intensities and structure determination, structure factor and its relation to electron density and intensity, Phase problem. Indexing of lattice planes in a cubic system, structure of NaCl and KCl, Avogadro's number from cubic lattice dimensions, applications of x-ray diffraction.

**Electron diffraction:**

Scattering of electrons by gases, Weir equation, experimental methods: visual method, sector, method, radial distribution method, low energy electron diffraction, structure determination of SiF<sub>4</sub> and CF<sub>3</sub>Cl, limitations. **Neutron diffraction:** Introduction, difference between neutron and x-ray diffraction measurement technique, magnetic scattering, applications, comparison of x-ray and neutron diffraction patterns for transition metal oxides

**Unit-V Radiochemical and Automated Methods of Analysis****12 hrs**

Radioactive Nuclides, Instrumentation, Neutron activation methods, Isotope dilution methods Automated Methods of Analysis: Overview, Flow – injection Analysis, Microfluidics, Discrete automatic systems

**Reference Books:**

1. Principles of Instrumental Analysis–Holler, Skoog & Crouch 6<sup>th</sup> edition
2. Instrumental Methods of Analysis–Willard, Merritt, Dean & Settle.
3. Principles of Instrumental Analysis–Skoog, F.J.Holler & J.A.Nieman
4. Instrumental Methods of Chemical Analysis–Galen W. Ewing.
5. Analytical Chemistry – Gary D. Christian, 6<sup>th</sup> edition
6. Handbook of Instrumental Techniques for Analytical Chemistry –Frank Settle, Editor
7. Introduction to Instrumental Analysis–R.D. Braun, McGraw Hill.
8. Fundamental of Analytical Chemistry, -D.A. Skoog, D.M. West and F.J. Holler.
9. Wilson and Wilson Comprehensive Analytical Chemistry. Ed. G. Svehla, A series of volumes.
10. Instrumental methods of analysis – Chatwal and Anand.
11. Instrumental methods of analysis – B. K. Sharma.

**Unit-I Polymer analysis****12 hrs**

Brief history to polymer, classification of polymer, how polymer are made.

Analysis and testing of polymer:

- a. Chemical analysis of polymer:  
X-ray diffraction analysis, thermal analysis, TGA, DTA.
- b. Physical testing of polymers:  
Mechanical properties, Fatigue testing, impact testing, tear resistance, hardness, abrasion resistance.
- c. Thermal properties: Softing temperature, flammability.
- d. Optical properties: Transmittance, color, gloss, haze and transparency.
- e. Electric properties: Dielectric constant and loss factor, resistivity, dielectric strength, electronic properties.
- f. Chemical properties: Resistance to solvents, vapor permeability, weathering.

**Unit-II Polymer analysis-molecular weight and size measurement****12 hrs**

Kinetics of polymerization, Molecular mass, Number and mass average molecular mass, Molecular mass determination by osmometry, Viscometry, light scattering and Sedimentation methods, End group analysis, colligative properties measurements, solution viscosity and molecular size, Numericals

**Unit-III Analysis of Paints and Pigments****12 hrs**

Introduction, Determination of non-volatile and volatile components, Flash point, Separation of pigments and thinner of solvent type coating, Pigment type, Identification of binders, Analysis of Vehicle and drying oils,

Analysis of pigments: Classification of organic and inorganic pigments, White tinted pigments.

**Unit-IV. Fuels:-****12 hrs**

Introduction, calorific value. Determination of calorific value. Modern concept of fuels.

Classifications of fuels, criterion of selection of fuels, properties of fuels. Method of processing.

Solids fuels, Natural solid fuels, Artificial solid fuels, Industrial solids fuels. Formation of coal properties of coal, Classification of coal, coking and non-coking coals. pulverised coal. Role of sulphur and ash in coal, approximate analysis, Ultimate analysis. Numerical.

**Unit-V Petroleum:-****12 hrs**

Occurrence, mining of petroleum. Prospecting colour and consistency. Origin composition, classification, terms related to petroleum. Distillation of crude petroleum. Treatment of the residual liquid, Determination of flash point. Determination of aniline point. Knocking and Anti-knocking compounds. Octane number. Cetane number, Numericals.

Gases fuels: Analysis of natural gases, liquefied petroleum gas, coal gas, water gas, producer gas, gobar gas, blast furnace gas and their calorific value determination.

Petrochemical analysis: Analysis of naphtha and their feed stocks, characterization of the catalyst used for cracking

**Reference Books:-**

1. Text Book of polymer science By F.W. Billmeyer, New York: Wiley
2. Physical polymer science by L.H. Sperling wiley – Interscience New York
3. Fundamentals of polymer science & Engineering By A Kumar & S.K. Gupta, Tata mcgraw Hill
4. Introduction to polymer science, V.R. Gowarnikar, N.V. Vishwanathan & J.
5. Industrial Chemistry, B. K. Sharma, Goel publishing House Meerut.
6. Kent, Rieg's Industrial chemistry, Rain hold.
7. Handbook of Instrumental Techniques for analytical chemistry. Frank Settle, editor
8. Polymer science by Vasant Govarikar, Wiley Earstewen. New York.
9. Principle of polymer science, Behadhar and Sastri, Narosa Publishing house.



**Name of experiment.**

1. Determination of COD, BOD and dissolved oxygen from waste water sample.
2. Separate and estimate the amount of cadmium and zinc using ion exchange resin.
3. Estimation of Nitrogen from given sample of fertilizer by Kejjaldal method.
4. Determination of saponification, acid and Iodine value of oil.
5. Determination Vitamin –C from given sample of Juice/ tablet using dichlorophenol indophenols by volumetric method.
6. Estimation of blood glucose by Folin Wu method.
7. Estimation of API in the pharmaceutical sample.
8. Estimation of phenol/aniline by bromination method.
9. Estimation of chloride from food sample by Volhard titration method.
10. Determination of sodium carbonate in washing soda.
11. Determination of volume strength of commercial hydrogen peroxide using  $\text{KMnO}_4$
12. Moisture content in pharmaceutical/food sample by Karl-fisher titration method.
13. Estimation of pesticide residue by TLC method.
14. Estimation of active chlorine in the given sample of bleaching powder.
15. Estimation of mg from given sample of talcum powder.
16. Estimation of alcohol in the given sample by diffusion oxidation method

**Reference Books**

1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogels.
2. Experiments in chemistry by D. V. Jahagirdar, Himalaya publication.
3. Practical Pharmaceutical Chemistry, 4th Ed. part-2, Beckett, Stenlake.
4. Indian Pharmacopeia volume –I , II III

**Name of experiment.**

1. Estimation of potassium, calcium and sodium from given sample using flame photometric method.
2. Determination of boric acid by conductometric method.
3. Determination of commercial vinegar by potentiometric titration and its confirmation by conductometric method.
4. Determination of molecular weight of high polymer by viscosity measurement /turbidometric method
5. Determine the amount of phosphate from given sample of fertilizer/ detergent using spectrophotometric method.
6. Estimation of Cu (II) and Fe (III) by spectrophotometric method using EDTA .
7. Estimate the reducing sugar by 3, 5 dinitrosalicylic acid in the given food sample by Spectrophotometric method.
8. Determination of protein by biureate method using by Spectrophotometric method.
9. Determine the percentage composition of the mixture by refractometer.
10. Characterization of unknown sample by IR Spectroscopy.
11. Analysis of mixture of alcohols by Gas chromatography.
12. Monitoring of nitration of organic compound by gas chromatography.
13. Determination of petroleum hydrocarbons in burn-cases by GC method.
14. Determine the lactose sugar by HPLC method
15. Analysis of binary mixture of simple organic compound by HPLC method.
16. Determine the Hammett constant of substituted benzoic acid by pH metric method.

**Reference Books**

1. Quantitative Inorganic Analysis including Elementary Instrumental Analysis by A. I. Vogels.
2. Experiments in chemistry by D. V. Jahagirdar, Himalaya publication.
3. Practical Pharmaceutical Chemistry, 4th Ed. part-2, Beckett, Stenlake.
4. Indian Pharmacopoeia volume –I, II & III

**Part – I Name of experiment**

1. Estimate the amount of copper and Tin from bronze alloy
2. Estimate the amount of lead and Tin from solder alloy
3. Estimate the amount of copper and Nickel from coin
4. Estimate the amount of copper and Zinc from brass alloy
5. Estimate the amount of Iron, Tin from hematite ore.
6. Estimate the amount of calcium, Magnesium and silica material from dolomite ore.
7. Estimate the amount of SiO<sub>2</sub>, calcium Iron Magnesium and aluminum from cement.
8. Determine the amount of Nickel and Iron from NiFe<sub>3</sub>O<sub>4</sub> ferrite sample

**Part B- Analytical Data interpretation and Structure Elucidation**

- i. UV Visible, IR, PMR, CMR mass Spectrum of organic and inorganic compounds.
- ii. XRD data analysis of organic and inorganic compounds
- iii. TGA, DTA data analysis of inorganic compounds
- iv. Different chromatograms.

**References books for CHEA422-to 424**

1. Systematic experimental physical chemistry – S. W. Rajbhoj & T. K Chondhekar
2. Quantitative Inorganic Analysis including Elementary Instrumental Analysis  
by A. I. Vogel's, 3rd Ed. ELBS (1964)
3. Standard methods of chemical analysis by F. J. Welcher
4. Indian Pharmacopeia volume –I , II III
5. British pharmacopeia.
6. Experiments in chemistry by D. V. Jahagirdar, Himalaya publication
7. Practical Pharmaceutical Chemistry, 4th Ed. part-2, Beckett, Stenlake
8. Standard Instrumental methods of Chemical Analysis, F. J. Welcher

**CHECA-401**  
**Analytical Method Development and Validation**

**30 hrs.**

**Credits: 02**

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**Unit-I Assay Validation and Inter Laboratory Transfer**

**15hrs**

Introduction, fundamental definitions, Essential principles of method transfer, method validation report, the inter-laboratory qualification (ILQ) process,

**Statistical Analysis and analytical Figure of Merit**

validation parameters: Accuracy, precision, calibration, (linear response functions (linear regression-errors in slope and the intercept, error in the estimate of concentration, standard additions), non-linear response functions and weighted regression analysis, internal standards), selectivity and specificity (chromatographic methods), limits of detections (spectrophotometric methods, chromatographic methods and related techniques, receptor binding assay), limit of quantification, sensitivity, ruggedness and robustness, analyte stability in the sample matrix, how to reduce systematic errors, mean and standard deviation, reliability of results, confidence interval, comparison of results, comparison of two means of two samples, experimental design

**Unit-II**

**15hrs**

**Overview of World Wide Regulations**

**Specific methods and Applications: Dissolution Studies**

Introduction, Dissolution test, Apparatus – USP type –I and II, Sampling and analytical instrumentation, Single point test Vs. Dissolution profile, Calibration, regulatory guidelines, analytical validation, linearity, accuracy, precision, specificity.

**Reference**

1. Development and validation of Analytical Methods, Progress Pharmaceutical and Biomedical Analysis, Vol-3, Edited by Chitofer M. Riley and Tomas W. Rosanske (Elvier)
2. Vogel's Textbook of quantitative Chemical Analysis, sixth Ed., Mendham, Denney, Barnes, Thomas, Pub: Pearson Education.
3. Handbook of modern pharmaceutical analysis, edited by Satinder Ahuja and Stephen Scypinski, Academic Press, Separation science Series, Vol-3
4. HPLC method Development for pharmaceuticals, Edited by Satinder Ahuja and Henrik Rasmussen, Academic Press, Separation science Series, Vol-8
5. Practical HPLC method Development, Snyder, Kirkiand, Glajch, Wiley India Pvt. Ltd.

**Unit-I Pharmaceutical Analysis-I****12 hrs.**

General idea regarding pharmaceutical industry, Definition and classification of drugs, types of dosage forms. Introduction to pharmaceutical formulations, Sources of impurities in pharmaceutical chemicals, raw materials & Products, Shelf life of pharmaceutical product and its determination, stability studies Standardization of finished products & their characteristics, Limit tests of As, Hg, Pb, Fe, Chlorides, and sulphates. Solubility tests, dissolution test, disintegration tests.

**Unit-II Pharmaceutical legislation****12 hrs.**

Introduction to drug acts, drug rules, FDA ISI, Agmark and other standard for pharmaceuticals & cosmetics particularly w.r.t. the testing of drugs, and raw material concerned. Pharmaceutical standards IP/BP/USP//EP. Cosmetic standards, Documentation, Record Keeping. Contents of labels, Types of packaging materials, Intellectual property rights: Introduction, role of patents in the pharmaceutical industry, recent changes, some case studies.

**Unit- III Pharmaceutical Analysis-II****12hrs**

Assay

of main classes of drugs as per IP with reference to Introduction, Type, Properties, Mode of action and Methods of Analysis.

**Unit-IV Forensic Analysis****12 hrs.**

Introduction, Special features of forensic analysis, Sampling, Sample storage, Sample dissolution. Toxicology: Classification of poisons and poisoning, Lethal Dose, Significance of LD50 and LC50. Extraction methods in toxicology: Isolation, Identification and determinations of: Narcotics: Heroin, Morphine, Codeine. Stimulants: Caffeine, Cocaine, Amphetamines. Despressant: Benzodiazepines- Diazepam, Oxazepam, Nitrazepam. Barbiturates- Phenobarbitone, Amylobarbitone, Pentobarbitone, Thiopentone. Hallucinogens: LSC and Cannabis. Analysis of biological stains and materials including blood, semen and saliva (qualitative and quantitative). Viscera, Stomach wash, Vomit and post mortem blood for poisons like cyanides, As, Hg, Insecticides and Pesticides.

**Unit-V Explosive:****12 hrs.**

Explosion, Detonation, Classification of explosives, Propellant, Fulminates, Detonators, Blasting-cap, Thermochemistry, Hygroscopicity of explosives, Moisture by Karl-Fisher titration, Isolation from debris, Qualitative test, Cation & anion analysis by capillary electrophoresis, EDXRF, Analysis by TLC, HPLC, IR, GC-TEA method.

**Reference Books:**

1. Isolation and Identification of drug-n E. G. Clarke vol.- I
2. Laboratory procedure manual-Forensic Toxicology- Directorate of forensic science, MHA Govt. of India.
3. Analytical Biochemistry, D. J. Holme and H. Peck, Longman
4. Bioanalytical Chemistry, S.R. Mikkelsen and E. Corton, John Wiley and Sons.
5. Immunoassay – a practical guide Eds, D.W. Chan and M.T. Perlstein, Academic Press.
6. Hawk's Physiological Chemistry, McGraw Hill.
7. Pharmaceutical Analysis Edited by David C. Lee, and Michael Webb.
8. Biochemical methods, S. Sadasivam, A. Manickam.
9. Standard Methods of Biochemical Analysis, S.R. Thimmaiah

**Unit-I Air Pollution**

**[12 hrs]**

General considerations: polluted air, Types of pollution and units of measurements. Air quality standards, Sampling, Monitoring, Analysis of CO, Sources and sinks of CO pollution, Effects of CO on plants and humans, Control of CO pollution, Analysis of oxides of nitrogen, NO<sub>x</sub> sources and sinks of NO<sub>x</sub> pollution, Control of NO<sub>x</sub> pollution, Hydrocarbons and photochemical smog and its control, Analysis of hydrocarbon in exhaust gasses, Petrol and air, Sulphur di oxide sources, Analysis and control, Acid rain particulates and their effects on human and climate, Control of particulates.

**Unit-II**

**12 hrs.**

- a. Water Pollution:** Aquatic environment, Water pollutants, Sampling of water and its preservation Trace metals in water, Chemical speciation with special reference to Copper, Lead, Mercury and Arsenic. Water quality standards Water quality parameters.
- b. Oxygen Demanding Wastes:** Dissolved oxygen, Biological oxygen demand, Monitoring techniques and methodology with special reference to ammonia, Nitrates, Nitrites, Fluorides, Cyanides, Total hardness, Lead, Cadmium and Mercury. Detection and control of Detergents, oils, Pesticides, Sewage treatment.

**Unit-III**

**12 hrs.**

- a) Chemical toxicology: Toxic** chemicals in environment, Impact of toxic chemicals on enzymes, Biochemical effects of Arsenic, Cadmium, Lead, Mercury, Carbon monoxide, Sulphur dioxide, Pesticides and Carcinogens.
- b) Soil analysis:** Sampling of soil, Determination of water holding capacity, Determination of total nitrogen, Ammonia and nitrates. Determination of Na, Mg, Ca, K, phosphate and Sulphur in soil.

**Unit-IV**

**12 hrs.**

**Industrial pollution:** Pollution due to cement industry, Distillery, Pharmaceutical (Drug) industries, Sugar industry, Paper and pulp industries, Thermal power plants, Nuclear power plants, Metallurgical industries, Polymer industries. Recycle, reuse, recovery, disposal, and management of solid industrial waste.

**Noise pollution-** Introduction, sources, measurement of noise level, differences between sound and noise pollution, reverberating of sound, effect and control

**Unit-V :**

**12 hrs.**

**Green Analytical Chemistry:** Principle and concepts of Green Chemistry: Sustainable development and green chemistry. Green analytical chemistry: Concept and trends, 'Greening' sample treatment: Reduced and solvent-free sample preparation methodologies, alternative solvents, energy saving procedures of analysis.

Green instrument analysis: Assessment of analytical methods for 'Greenness', greening flow injection analysis, chemical sensors, liquid green chromatography

**Reference Books:**

1. A. K. De, Environmental Chemistry, Wiley Eastern Ltd. New Delhi.
2. S. L. Chopra and J. S. Kanwar, Analytical, Agricultural Chemistry, Kalyani Publishers,
3. R. K. Trivedy and P. K. God, Chemical and biological methods for water pollution studies, Environmental publications, co. New Delhi.
4. L. A. Richards, Diagnosis and improvement of saline and alkali soils. Oxford IBH publications co. New Delhi.
5. S. M. Khopkar, Environmental chemistry, Environmental pollution analysis
6. Environmental chemistry-B.K. Sharma. Goel publishing house Meerut
7. M. S. Creos and Morr, Environmental chemical analysis, American publications.
8. M. Sitting, Resources, Recovery and Recycling, Handbook of industrial waste.

9. Standard methods of water and waste water analysis, American public health association Washington D. C.
10. R. Gopalan and Amrutha Anand, "Environmental chemistry laboratory manual Emerald Publication.
11. Standards for water for drinking and other purposes, Beaurau of Indian Standards India.
12. Guideline for drinking water quality recommendations of world health organization, Geneva.
13. B. K. Sharma and H. Kaur, Environmental Chemistry, Goel publishing house Meerut.
14. Thomas G. Spiro and Willian M. Stigliani, Chemistry of environment.
15. New Trends in green Chemistry, V.K.Ahluwalia and M. Kidwai, Anamaya Publishers New Delhi, (2004)

**Unit-I General concepts of food analysis.****12 hrs**

Nutrient value of food.

Physical characteristics &amp; chemical constituents

Proximate composition of food

Legislation related to food and recent amendments, Standards and public health

a) General idea regarding food processing and preservation

b) Food contamination and spoilage

c) Food safety considerations.

d) Adulteration-Introduction, Types, Tests for adulterants, control

**Unit-II Analysis of food-****12 hrs**

a). Study of followings with their estimation methods : Food preservatives, Food emulsifiers, Food stabilizers, Food thickener,

b). Introduction, Standard composition and Analysis of the following foods: Milk and milk products, Tea, Coffee, Cereals &amp; Flour, Honey, Soft drinks &amp; Alcoholic beverages.

**Unit- III Analysis of Oils, Fats Soap and Detergents****12 hrs**

Introduction to natural oils and fats, Analysis of oils and fats, Softing point, Congent point, Titer point, Cloud point, Iodine, Saponification, acid, Hydroxyl, R-M and polenske values, Elaiden test.

Introduction to soaps, Analysis of soaps, for saponification, Unsaponifiable and unsaponified matter in soaps, Estimation of free alkali and phenol in soap, Classification of detergents (in Brief),

Analysis of active ingredients from detergents (methelene blue and hyamine 1622 method), Estimation of CMC, Chlorides, Total phosphates

**Unit-IV****12 hrs**a) **Analysis of fertilizers.** Classification of fertilizer, NPK value, Chemical composition of superphosphate, Lime and Potash fertilizer, Analysis of commercially available fertilizers for N, P & K.b) **Analysis of pesticides.** : Legislation and recent amendments with respect to pesticides materials. Names of pesticides and their chemical structures. , Application dosage of different pesticides. , Analysis of specific pesticides.**Unit-V Analysis of Vitamins****12 hrs**Analytical techniques of determination of water and fat soluble vitamins including microbiological techniques. **Human nutrition:** Biological values and estimation of enzymes, Carbohydrates, essential amino acids, proteins and lipids.**Reference Books:-**

1. Chemical analysis of food By Pearson.
2. Introductions to food science and technology, series by G.F.Stewart and M.A.Amerine Academic process.
3. Applied chemistry .A Text book for Engineers and technologists by H.D.Gesser.
4. Food analysis by Nielson.
5. Food additives by S.N.Mahindry (APH) publication
6. Jacob (M.B) chemical Analysis of food and food products ( Van Nostrand co. New York)
7. Analytical chemistry of foods (C.S.James) Blackie Academic and professional
8. Food Analysis principles and techniques D.W.Gruenwedel, J.R. Whitaker, MercelDekker
9. Food analysis Theroy and practice Y.pomeranz and C.E.Meloan, Chapman and Hill
10. Food Analysis ,2<sup>nd</sup> edition S.S Nelsen, Aspen publishers
11. Food analysis, A. G. Woodman, McGraw Hill



**Unit-I Analysis of ores**

**12hrs**

Composition and analysis of Dolomite, Bauxite, Ilminite, Zinc blend, hematite, pyrolusite and calcite for their major constituents using one of the standard methods of analysis.

**Unit-II Analysis of alloys**

**12 hrs**

Composition, Properties, uses and analysis of : Brass, Bronze Solder, Stainless Steel, Monel-metal, gun-metal, Silver coin for their major constituents using one of the standard methods of analysis

**Unit-III Analysis of Cement and building materials**

**12 hrs**

Types of cement, Sampling, Analysis of- Silicon dioxide, Aluminum oxides, Ferric oxides, Calcium oxide, Magnesium oxide, Sodium and potassium oxide.

**Analysis of Glass:** Types of glasses, Determination of lead and lead glass.

**Unit-IV Cosmetic Analysis.**

**12 hrs**

- a) Introduction to cosmetics.
- b) Evaluation of cosmetic materials-raw materials, additives, colours, perfumes.
- c) Legislation and recent amendments with respect to cosmetic materials.
- d) Analysis of Physical and chemical constituents of : Skin powder , Creams , Lipsticks , Lotions

**Unit-V Analysis.of wood, pulp and paper**

**12 hrs**

**Wood:** sampling, determination of methoxy group in wood. A brief idea of analysis of moisture in wood chips and saw dust by toluene methods, cellulose in wood.

**Pulp:** Introduction, sampling, determination of cellulose in pulp, permanganate number of pulp, copper number of pulp.

**Paper:** Introduction,sampling,determination of reducible Sulphur in paper and paper boards, moisture in paper, ash in paper, starch in paper, cellulose in paper, copper number of paper, acid-soluble iron in paper

**Reference books.**

1. Hillenbrand Lhundel, Bright and Hoffman, Applied inorganic analysis, John Wiley.
2. Snell and Biffen, Commercial methods of analysis.
3. P. G. Jeffery, Chemical methods of rock analysis, pergamon.
4. Rieche, Outline of industrial organic chemistry, Butter worth.
5. Kent, Rieg's Industrial chemistry, Rain hold
6. P. G. Jeffery and. J. Hatchinson, Chemical methods of rock analysis.
7. F. J. Welcher Standard methods of chemical analysis, a series of volume Robert and Krigeeger Publishing Company.
8. Metallurgical analysis by S. K. Jain and K. K. Jain.

**Unit-I Microbial Analysis.**

**15hrs**

- a) Introduction to Microbiology, Application to pharmacy, Study of different types of micro-organisms( Bacteria, Viruses, and Fungi) w.r.t. morphology, cell characteristics, habits, nutrition, reproduction, and cultivation
- b) Isolation of important groups of bacteria by- Total viable count, Standard plate count.
- c) Microbial growth and factors affecting it: Temperature, pH, Heavy metals (media), Relative humidity, Molecular oxygen and Osmotic pressure.
- d) Sterilization-Principle, Methods used in general and as applied to Pharmaceutical products.
- e) Disinfectants-Classification, mode of action, efficiency.

Antiseptic techniques: Sterility tests for typical Pharmaceutical products

**Unit-II - Clinical Analysis**

**15 hrs**

Introduction: Body fluids: Composition, Collection and Preservation of body fluids and detection of abnormal levels of certain constituents leading to diagnosis of diseases and disorders. Analysis of constituents of physiological fluids, 1.Blood -PH, Glucose, Urea. 2.Serum-uric acid, total protein, albumin, globulin& A/G ratio, barbiturates, alkaline phosphatase, acid phosphatase, bilirubin, cholesterol, amylase, creatinine carbohydrates.. Urine- Immunological methods: General process of immune response, Antibody-Antigen ratio, Precipitation reactions, Enzyme linked-immunosorbent assays ELISA

**Unit-III Determination of vitamins in body fluid**

**15 hrs**

Classification of vitamins with example, Each vitamin must be explained with respect of functions, deficiency diseases, daily requirement, and analytical method i) Retinol (determination of retinol and serum carotene in serum using TFA), Vit D3 (cholecalciferol), Vitamin E (Tocopherols, Determination of serum tocopherol by spectrophotometry by dipyrindyl method), Vitamin B1 (thiamine determination by flurometry), Vitamin B2 (riboflavin, Photofluorometric method), Vitamin B6 (Pyidoxine, Fluorometric determination of Xanthuric acid), Nicotinic acid and Niacin: determination by fluorometry, Ascorbic acid (vitamin -c) Volumetric method using 2,6 dichlorophenol method, colorimetric determination of leucocyte ascorbate.

**Unit-IV Enzyme catalysis Analytical applications**

**15 hrs**

Basic principles, catalysis-measurement of catalytic reactions, nonspecificity of catalysts, types of reactions catalyzed, enzyme catalysis,enzyme kinetics, properties of enzyme, enzyme inhibitors and activators, enzyme specificity, determination of enzymes and enzyme substrates, Examples of enzymatic analysis dehydrogenase reactions, substrate determinations: glucose, uric acid.Immobilized enzymes, Evaluation methods.

**Reference Books:**

1. General Microbiology- R. V. Stainer 6<sup>th</sup> edition
2. Principle of microbiology- A. J. Salle
3. Microbiology- Pleczar
4. An Introduction to Practical Biochemistry, David Plummer.
5. Biochemical methods, S. Sadasivam, A .Manickam
6. Standard Methods of Biochemical Analysis, S.R. Thimmaiah

**CHEAR-407: Research project (Experimental)**

**24 Hrs/week**

**Credit: 12**

**200 Marks**

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**Tentative topic for projects**

**Projects to be based upon convenient analytical protocol for analysis of one of the following materials**

- a. Drugs/ Medicines
- b. Dyes/ Paints/ cosmetics
- c. Milk product/ vegetable oils/ beverages
- d. Plastics and polymers
- e. Ores & alloys
- f. Fertilizer, insecticide, Pesticide
- g. Environmental samples , air, water, soil
- h. Any other material other than above.

**Scheme of marking**

**Project work Evaluation: 25 marks**

- i. Literature survey
- ii. Experimental procedures, photographs
- iii. Characterizations techniques: Fundamentals principles of respective techniques
- iv. Spectrum / images of prepared materials
- v. Data analysis / applications of synthesized materials
- vi. Conclusion
- vii. Reference citations
- viii. Holistic response of students (scientific thinking, power of imagination, Punctuality, efforts, curiosity.)

**Power point presentation of Project work: 25 marks**

- i. Self-preparation PPT
- ii. Skill of presentation
- iii. Contents of presentation
- iv. Subject knowledge
- v. Manuscript preparation/acceptance/publication

**Reference: Internet search**

**CHEAR-408 : Research project (Dissertation, Presentation and Seminars)**

**6 Hrs/week**

**Credit: 6**

**100 Marks**

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1. Isolation and Identification of drug-n E. G. Clarke vol.- I
2. Laboratory procedure manual-Forensic Toxicology- Directorate of forensic science, MHA Govt. of India.
3. Pharmaceutical Analysis Edited by David C. Lee, and Michael Webb.
4. Biochemical methods, S. Sadasivam, A .Manickam.
5. Standard Methods of Biochemical Analysis, S.R. Thimmaiah
6. Pearson's Composition and analysis of food.- Ronald S.Kirk and Ronald Sawyer.
7. Introductions to food science and technology, series by G.F.Stewart and M.A.Amerine Academic process.
8. Applied chemistry .AText book for Engineers and technologists by H.D.Gesser.
9. Food analysis by Nielson.
10. Food additives by S.N.Mahindry (APH) publication
11. Jacob (M.B) chemical Analysis of food and food products ( Van Nostrand co. New York)
12. Analytical chemistry of foods (C.S.James) Blackie Academic and professional
13. Food Analysis principles and techniques D.W.Gruenwedel, J.R.Whitaker, MerceDekker
14. Food analysis Theroy and practice Y.pomeranz and C.E.Meloan,Chapman and Hill
15. Food Analysis ,2<sup>nd</sup> edition S.S Nelsen, Aspen publishers
16. Food analysis, A. G. Woodman, McGraw Hill