

JSS Mahavidyapeetha

JSS COLLEGE OF ARTS, COMMERCE AND SCIENCE

B. N. ROAD, MYSURU – 570 025

POSTGRADUATE DEPARTMENT OF CHEMISTRY
SYLLABUS FOR M.Sc. DEGREE PROGRAMME

CHOICE BASED CREDIT SYSTEM

2017-2018

CHEMISTRY IN A NEW LIGHT

Analytical

Inorganic

Organic

Physical

CHEMISTRY



GENERAL REQUIREMENTS

Scheme of Instructions:

- A. A Masters Degree program is of 4 semesters-two years duration. A candidate can avail a maximum of 8 semesters – 4 years (in one stretch) to complete Masters Degree (including blank semesters, if any). Whenever a candidate opts for blank semesters, he/ she has to study the prevailing courses offered by the department when he/ she continues his/ her studies.
- B. A candidate has to earn a minimum of 76 Credits, for successful completion of a Master Degree. The 76 Credits shall be earned by the candidate by studying Hard Core, Soft Core and Open Elective.
- C. **Minimum for Pass:** In case a candidate secures less than Thirty percent in C₁ and C₂ put together, the candidate is said to have DROPPED the course, and such a candidate is not allowed to appear for C₃.
- D. In case a candidate secures less than Thirty percent in C₃, or secures more than Thirty percent in C₃ but less than Thirty percent in C₁, C₂ and C₃ put together, the candidate is said to have not completed the course and he/ she may either opt to DROP the course or to utilize PENDING option.
- E. **Credits (Minimum) Matrix:** A candidate has to study a minimum of 16 Credits in Soft Core (sum total of 4 semesters) and 04 Credits in Open Elective (in III Semester) for the successful completion of the Masters Degree course. A minimum of 15 students should register for every Soft Core or Open Elective course.
- F. All other rules and regulations hold good which are governed by the College/ University.

GENERAL SCHEME WITH RESPECT TO THE ASSESSMENT OF CREDITS

Semester	Hard Core (HC)		Total	Soft Core (SC)		Total	Open Elective (OE)
	Theory	Practicals		Theory	Practicals		
I	3+3+3+3=12	(4+4)+(4+4)=08 ^a	20	2+2+2+2=08 ^b	NIL	08^b	NIL
II	3+3+3+3=12	(4+4)+(4+4)=08 ^a	20	2+2+2+2=08 ^b	NIL	08^b	NIL
III	3+0+3+0=06	NIL	06	0+(2x2)+0+(2x2)=08	(4+4)+(4+4)=08 ^{a,c}	16	04
IV	0+3+0+3=06	NIL	06	(2x2)+0+(2x2)+0=08	4 ^d +(4+4)+(4+4)=08 ^{a,c}	18	NIL
Grand Total	36	16	52	26	16	42	04

^aFifty percent of the students will attend Analytical/ Inorganic Practical and remaining Fifty percent students will attend Organic/ Physical Practical in I or III Semester and *vice-versa* during II or IV Semester.

^bCourses are common for both I and II Semesters and the candidate can opt any course of his/ her choice in aforesaid semesters and should ascertain that the course/ s already studied in I Semester are not repeated in the II Semester.

^cPracticals are only for chemistry students which are compulsory courses.

^dDissertation/ Project work

SCHEME OF STUDY AND EXAMINATION

FIRST SEMESTER HARD CORE

THEORY

Course	Title	Contact Hours/Week	Credits	Max. Marks/Course	Internal Assessment Marks		Semester End Exams (C ₃)	
					C ₁	C ₂	Duration	Max. Marks
CHA HCT: 1.1.	Fundamentals of Chemical Analysis	03	03	100	15	15	03	70
CHI HCT: 1.2.	Inorganic Chemistry-I	03	03	100	15	15	03	70
CHO HCT: 1.3.	Stereochemistry; Molecular Rearrangements and Heterocyclic Chemistry	03	03	100	15	15	03	70
CHP HCT: 1.4.	Physical Chemistry-I	03	03	100	15	15	03	70

PRACTICALS

Course	Title	Contact Hours/Week	Credits	Max. Marks/Course	Internal Assessment Marks		Semester End Exams (C ₃)	
					C ₁	C ₂	Duration	Max. Marks
CHA HCP: 1.5.	Analytical Chemistry Practicals	08	04	100	15	15	06	70
CHI HCP: 1.6.	Inorganic Chemistry Practicals	08	04	100	15	15	06	70
CHO HCP: 1.7.	Organic Chemistry Practicals	08	04	100	15	15	06	70
CHP HCP: 1.8.	Physical Chemistry Practicals	08	04	100	15	15	06	70

Note: Fifty percent of the students will attend Analytical and Inorganic practicals and remaining Fifty percent of the students will attend Organic and Physical practicals in I semester and *vice-versa* during II semester.

SOFT CORE

THEORY

Course	Title	Contact Hours/Week	Credits	Max. Marks/Course	Internal Assessment Marks		Semester End Exams (C ₃)	
					C ₁	C ₂	Duration	Max. Marks
CHA SCT: 1.1.	Applied Analysis I	02	02	100	15	15	03	70
CHI SCT: 1.2.	Frontiers in Inorganic Chemistry	02	02	100	15	15	03	70
CHO SCT: 1.3.	Reaction Mechanisms	02	02	100	15	15	03	70
CHP SCT: 1.4.	Solid State Chemistry and Chemistry of Nano Materials	02	02	100	15	15	03	70

SECOND SEMESTER HARD CORE

THEORY

Course	Title	Contact Hours/Week	Credits	Max. Marks/Course	Internal Assessment Marks		Semester End Exams (C ₃)	
					C ₁	C ₂	Duration	Max. Marks
CHA HCT: 2.1.	Separation Techniques	03	03	100	15	15	03	70
CHI HCT: 2.2.	Advanced Coordination Chemistry	03	03	100	15	15	03	70
CHO HCT: 2.3.	Reagents in Organic Synthesis; Photochemistry and Pericyclic Reactions	03	03	100	15	15	03	70
CHP HCT: 2.4.	Physical Chemistry - II	03	03	100	15	15	03	70

PRACTICALS

Note: It is same as that of I Semester. Students who have studied Analytical/ Inorganic or Organic/ Physical Practicals will get interchanged during II Semester.

SOFT CORE

All the courses are common for both I and II Semesters and the candidate can opt any course of his/ her choice in aforesaid semesters and should ascertain that the course/ s already studied in I Semester are not repeated in the II Semester

THIRD SEMESTER

HARD CORE

THEORY

Course	Title	Contact Hours/Week	Credits	Max. Marks/Course	Internal Assessment Marks		Semester End Exams (C ₃)	
					C ₁	C ₂	Duration	Max. Marks
CHA HCT: 3.1.	Instrumental Methods of Analysis	03	03	100	15	15	03	70
CHO HCT: 3.2.	Spectroscopy	03	03	100	15	15	03	70

SOFT CORE

THEORY

Course	Title	Contact Hours/Week	Credits	Max. Marks/Course	Internal Assessment Marks		Semester End Exams (C ₃)	
					C ₁	C ₂	Duration	Max. Marks
CHI SCT: 3.1.	Inorganic Chemistry-II	02	02	100	15	15	03	70
CHI SCT: 3.2.	Structural Methods in Inorganic Chemistry	02	02	100	15	15	03	70
CHP SCT: 3.3.	Biophysical Chemistry and polymers	02	02	100	15	15	03	70
CHP SCT: 3.4.	Applications of Chemical Kinetics and Quantum Chemistry	02	02	100	15	15	03	70

PRACTICALS

Course	Title	Contact Hours/Week	Credits	Max. Marks/Course	Internal Assessment Marks		Semester End Exams (C ₃)	
					C ₁	C ₂	Duration	Max. Marks
CHA SCP: 3.5.	Analytical Chemistry Practicals	08	04	100	15	15	06	70
CHI SCP: 3.6.	Inorganic Chemistry Practicals	08	04	100	15	15	06	70
CHO SCP: 3.7.	Organic Chemistry Practicals	08	04	100	15	15	06	70
CHP SCP: 3.8.	Physical Chemistry Practicals	08	04	100	15	15	06	70

Note: 1. Fifty percent of the students will attend Analytical and Inorganic practicals and remaining Fifty percent of the students will attend Organic and Physical practicals in III semester and *vice-versa* during IV semester.

2. Practicals papers are only for chemistry students which are compulsory

OPEN ELECTIVE (for Non-Chemistry Students only)

Course	Title	Contact Hours/Week	Credits	Max. Marks/Course	Internal Assessment Marks		Semester End Exams (C ₃)	
					C ₁	C ₂	Duration	Max. Marks
CH OET	Selected Topics in Chemistry	04	04	100	15	15	03	70

FOURTH SEMESTER
HARD CORE

THEORY

Course	Title	Contact Hours/Week	Credits	Max. Marks/Course	Internal Assessment Marks		Semester End Exams (C ₃)	
					C ₁	C ₂	Duration	Max. Marks
CHI HCT: 4.1.	Bioinorganic Chemistry	03	03	100	15	15	03	70
CHP HCT: 4.2.	Advanced physical chemistry	03	03	100	15	15	03	70

SOFT CORE

THEORY

Course	Title	Contact Hours/Week	Credits	Max. Marks/Course	Internal Assessment Marks		Semester End Exams (C ₃)	
					C ₁	C ₂	Duration	Max. Marks
CHA SCT: 4.1.	Applied Analysis II	02	02	100	15	15	03	70
CHA SCT: 4.2.	Applied Analysis III	02	02	100	15	15	03	70
CHO SCT: 4.3.	Retrosynthesis and Organometallic Chemistry	02	02	100	15	15	03	70
CHO SCT: 4.4.	Biomolecules and Natural Products	02	02	100	15	15	03	70

PRACTICALS

Note: It is same as that of III Semester. Students who have studied Analytical/ Inorganic or Organic/ Physical Practicals will get interchanged during IV Semester.

SCHEME OF EXAMINATION FOR C₁, C₂ AND C₃ COMPONENTS

Preamble: In view of the CBCS syllabus, following is the model distribution of marks for C₁, C₂ and C₃ Components. At a glance, the model includes both theory (HC/ SC/ OE) as well as practicals (HC/ SC) assessment of marks.

The following is the scheme which will be followed for the assessment of marks for both theory (HC/ SC/ OE) as well as practicals (HC/ SC) irrespective of the Credits associated with each Course. Thirty percent of the marks will be assessed for the internals (C₁ and C₂) and remaining seventy percent will be for the semester end examinations (C₃). Each Course carries 100 marks and hence thirty marks for internal assessment and remaining seventy marks will be for Semester End Examinations. Out of thirty marks for internals, fifteen marks will be allotted to each C₁ and C₂ components. The distribution of marks for C₁ and C₂ varies with HC and SC papers.

Each theory Course (HC/ SC/ OE) consists of three components namely C₁, C₂ and C₃. C₁ and C₂ are designated as Internal Assessment (IA) and C₃ as Semester End Examination. Each Course (HC/ SC/ OE) carries **100 Marks** and hence the allotment of marks to C₁, C₂ and C₃ Components will be fifteen, fifteen and seventy marks respectively. i.e.,

C ₁ Component	: 15 Marks	} Internal Assessment Marks
C ₂ Component	: 15 Marks	
C ₃ Component	: 70 Marks	Semester End Examination
Total	: 100 Marks	

The above will be followed in common for all the theory (HC/ SC/ OE) and practical (HC/ SC) Courses in all the four semesters.

1. THEORY:

1.1. HARD CORE (03 CREDITS COURSES)

1.1.1 Distribution of Marks for C₁ and C₂ Components (I/ II Semesters):

IA consists of fifteen marks for each component it will be divided into three parts viz., *Internal Test, Home Assignment and Seminar*. Internal tests will be conducted during the 8th Week of the semester for C₁ and 16th Week of the semester for C₂. Home Assignment will be

concerned for C₁ Component and Seminar for C₂ Component only. Hence, a teacher may give only one assignment (or in their personal interest one more may be given). Since each Course has three units, the marks shall be divided equally. Allotment of marks for C₁ and C₂ is as follows: Out of fifteen Marks for IA for C₁, Internal test will be conducted for Thirty Marks (reduced to 10 Marks) and Home Assignment will be given for 05 Marks (Each Home Assignment from every unit will be assessed for 05 Marks and finally reduced to 05 Marks). IA for C₂ will be distributed as follows: Internal test will be conducted for Thirty Marks (reduced to 10 Marks) and Seminar will be assigned for 05 Marks for the favor of IA. Please note that actual Seminar will be assessed for 20 Marks and finally 05 Marks will be distributed to each theory HC Course. i.e.,

C ₁		C ₂	
Internal Test	: 30 Marks (10+10+10) Reduced to 10 Marks	Internal Test	: 30 Marks (10+10+10) Reduced to 10 Marks
Home Assignment	: 15 Marks (05+05+05) Reduced to 05 Marks	Seminar	: 20 Marks (05+05+05+05) Distributed 05 Marks to each HC Course
Total	: 15 Marks	Total	: 15 Marks

1.1.1a Distribution of Marks for C₁ and C₂ Components (III/ IV Semesters):

The modalities discussed above in 1.1.1 holds good for this also except for Seminar component. Seminar will be assigned for 05 Marks for the favor of IA. Please note that actual Seminar will be assessed for 10 Marks and finally 05 Marks will be distributed to each theory HC Course. i.e.,

C ₁		C ₂	
Internal Test	: 30 Marks (10+10+10) Reduced to 10 Marks	Internal Test	: 30 Marks (10+10+10) Reduced to 10 Marks
Home Assignment	: 15 Marks (05+05+05) Reduced to 05 Marks	Seminar	: 10 Marks (05+05) Distributed 05 Marks to each HC Course
Total	: 15 Marks	Total	: 15 Marks

1.1.2 Distribution of Marks for C₃ Component (Semester End Examination):

The question paper is of 3 hr duration with Max. Marks 70. The following question paper pattern will be followed for all the theory Courses (HC/ SC/ OE). Question paper will have 2 parts both parts will cover all units of the course with equal proportional of distribution. Part A is of Short Answer Type questions which will have ten questions and each question carries two Marks. Part B carries fifty Marks and comprises of seven questions where in a student has to answer any five. Each question carries ten marks with sub question i.e.,

Model Question Paper Pattern:

Max. Duration: 3 Hr

Max. Marks: 70

Note: *Question paper has two parts, answer both the parts.*

PART A

Ten questions will be given and all ten should be answered. Each question carries two marks.

10 x 2 = 20

PART B

Seven questions will be given and any five should be answered. Each question carries Ten marks. An examiner may distribute marks as (3+3+4), (5+5), (7+3) & (4+6). Two marks question shall be avoided to maximum extent.

5 x 10 = 50

1.2 SOFT CORE (02 CREDITS COURSES):

1.2.1 Distribution of Marks for C₁ and C₂ Components:

IA consists of 15 marks for each components; it will be divided into two parts viz., *Internal Test and Home Assignment*. Internal tests will be conducted during the 8th Week of the semester for C₁ and 16th Week of the semester for C₂. As far as Home Assignment is concerned, the concerned teacher will assign one or two Home Assignments to each student. Since each Course has two units, the marks will be divided equally. Allotment of marks for C₁ and C₂ is as follows: Out of 15 Marks for IA, Internal tests will be conducted for 10 marks and Home Assignment for 05 Marks. i.e.,

C ₁		C ₂	
Internal Test	: 20 Reduced to 10	Internal Test	: 20 Marks 10
Home Assignment	: 10 Marks Reduced to 05	Home Assignment	: 10 Marks Reduced to 05
Total	: 15 Marks	Total	: 15 Marks

1.2.2 Distribution of Marks for C₃ Component (Semester End Examination):

The above discussed pattern (1.1.2) holds good in this case also.

1.3 OPEN ELECTIVE (04 CREDITS COURSE):

1.3.1 Distribution of Marks for C₁ and C₂ Components:

IA consists of 15 marks for each components; it will be divided into two parts viz., *Internal Test and Home Assignment*. Internal tests will be conducted during the 8th Week of the semester for C₁ and 16th Week of the semester for C₂. As far as Home Assignment is concerned, the concerned teacher will assign one or two Home Assignments to each student. Allotment of marks for C₁ and C₂ is as follows: Out of 15 Marks for IA, Internal tests will be conducted for 20 marks and reduced to 10 Home Assignment for 05 Marks. i.e.,

C ₁		C ₂	
Internal Test	: 20 Marks Reduced to 10	Internal Test	: 20 Marks Reduced to 10
Home Assignment	: 20 Marks Reduced to 05	Home Assignment	: 20 Marks Reduced to 05
Total	: 15 Marks	Total	: 15 Marks

1.3.2 Distribution of Marks for C₃ Component (Semester End Examination):

The above discussed pattern (1.1.2) holds good in this case also.

2. PRACTICALS (04 CREDITS COURSES):

The following scheme will be applicable for both HC and SC in all the four semesters (SC courses are for chemistry students only which are compulsory Courses).

Each practical (HC/ SC) consists of three components namely C₁, C₂ and C₃. C₁ and C₂ are designated as Internal Assessment (IA) and C₃ as Semester End Examination. Each practical (HC/ SC) carries **100 Marks** and hence the allotment of marks to C₁, C₂ and C₃ Components will be fifteen, fifteen and seventy marks respectively. i.e.

C ₁ Component	: 15 Marks	} Internal Assessment Marks
C ₂ Component	: 15 Marks	
C ₃ Component	: 70 Marks	Semester End Examination
Total	: 100 Marks	

2.1 Distribution of Marks for C₁ and C₂ Components:

IA consists of **15 Marks**; it will be divided into three parts viz., *Internal Test, Continuous Assessment and Record*. Continuous assessment refers to the daily assessment of each student based on his/ her attendance, skill, results obtained etc. Thus, three marks are allotted for Continuous Assessment. Internal tests will be conducted for ten marks during the 8th Week of the semester for C₁ and 16th Week of the semester for C₂. Finally, remaining two Marks will be for the record. i.e.,

C ₁		C ₂	
Internal Test	: 10 Marks	Internal Test	: 10 Marks
Continuous Assessment	: 03 Marks	Continuous Assessment	: 03 Marks
Record	: 02 Marks	Record	: 02 Marks
Total	: 15 Marks	Total	: 15 Marks

5.1.2 Distribution of Marks for C₃ Component (Semester End Examination):

The end examination will be conducted for **seventy Marks/ Course** with a maximum duration of six hours. Two experiments will be given to each student which carries thirty Marks each. Each student will be subjected to Viva-Voce Examination for which ten Marks is allotted. i.e.,

Two Experiments	: 60 Marks
Viva-Voce	: 10 Marks
Total	: 70 Marks

2.3 Evaluation of Project Work/ Dissertation (Minor):

Each student can take up Project Work/ Dissertation under the guidance of the faculty of the department during the IV Semester as a Soft Core course.

2.3.1 Distribution of Marks for C₁ and C₂ Components:

IA consists of **fifteen Marks** for each components; it will be divided into three parts viz., *Attendance, Continuous Assessment and Work Progress*. Continuous assessment refers to the daily assessment of each student based on his or her skill, results obtained, literature survey etc. C₁ will be assessed during the 8th Week of the semester and C₂ during the 16th Week of the semester. Hence, the concerned guide will prepare the marks list based on the above said parameters for both C₁ and C₂ Components.

2.3.2 Distribution of Marks for C₃ Component (Semester End Examination):

The semester end examination will be conducted for **seventy Marks**. Every student is suppose to prepare a hard copy of the findings of the work in the form of report and submitted for evaluation. This part will be assessed for fourth Marks. Each student will be subjected to Viva-Voce Examination for which thirty Marks is allotted. i.e.,

Evaluation of Report	: 40 Marks
Viva-Voce	: 30 Marks
Total	: 70 Marks

FIRST SEMESTER

THEORY – HARD CORE

CHA HCT: 1.1. FUNDAMENTALS OF CHEMICAL ANALYSIS

UNIT – I

Analytical Chemistry - Meaning and analytical prospective, scope and function: Analytical problems and their solutions, trends in analytical methods and procedures.

Language of analytical chemistry - Analysis, determination and measurement. Techniques, methods, procedures and protocols. Classifying analytical techniques. selecting an analytical method - accuracy, precision, sensitivity, selectivity, robustness and ruggedness. Scale of operation, equipment, time and cost. Making the final choice

Errors and treatment of analytical data: Limitations of analytical methods – Error: determinate and indeterminate errors, minimization of errors. Accuracy and precision, distribution of random errors, the normal error curve. Statistical treatment of finite samples - measures of central tendency and variability: mean, median, range, standard deviation and variance. Student's t-test, confidence interval of mean. Testing for significance - comparison of two means and two standard deviations. Comparison of an experimental mean and a true mean. Criteria for the rejection of an observation - Q-test. Propagation of errors: determinate errors and indeterminate errors.

Standardization and calibration: Comparison with standards - direct comparison and titrations. External standard calibration - the least squares methods, regression equation, regression coefficient. Internal standard methods and standard-addition methods. Figures of merit of analytical methods - sensitivity and detection limit, linear dynamic range.

[16 HOURS]

UNIT – II

Obtaining and preparing samples for analysis: Importance of sampling, designing a sample plan-random, judgement, systematic-judgement, stratified and convenience sampling. Type of sample to collect - grab and composite samples. *In situ* sampling. Size of sample and number of samples. Implementing the sampling plan - solutions, gases and solids. Bringing solid samples into solution - digestion and decomposing.

Titrimetric analysis: An overview of titrimetry. Principles of titrimetric analysis. Titration curves. Titrations based on acid-base reactions - titration curves for strong acid and strong base,

weak acid and strong base and weak base and strong acid titrations. Selecting and evaluating the end point. Finding the end point by visual indicators, monitoring pH and temperature. Quantitative applications – selecting and standardizing a titrant, inorganic analysis - alkalinity, acidity and free CO_2 in water and waste waters, nitrogen, sulphur ammonium salts, nitrates and nitrites, carbonates and bicarbonates. Organic analysis - functional groups like carboxylic acid, sulphonic acid, amine, ester, hydroxyl, carbonyl. Air pollutants like SO_2 . Quantitative calculations. Characterization applications - equivalent weights and equilibrium constants.

Acid-base titrations in non-aqueous media: Role of solvent in acid-base titrations, solvent systems, differentiating ability of a solvent, some selected solvents, titrants and standards, titration curves, effect of water, determining the equivalence point, typical applications - determination of carboxylic acids, phenols and amines.

[16 HOURS]

UNIT – III

Precipitation titrations: Titration curves, feasibility of precipitation titrations, factors affecting shape - titrant and analyte concentration, completeness of the reaction, titrants and standards, indicators for precipitation titrations involving silver nitrate, the Volhard, the Mohr and the Fajan's methods, typical applications.

Complexometric titrations: Complex formation reactions, stability of complexes, stepwise formation constants, chelating agents, EDTA - acidic properties, complexes with metal ions, equilibrium calculations involving EDTA, conditional formation constants, derivation of EDTA titration curves, effect of other complexing agents, factors affecting the shape of titration curves - completeness of reaction, indicators for EDTA titrations - theory of common indicators, titration methods employing EDTA - direct, back and displacement titrations, indirect determinations, titration of mixtures.

Redox titrations: Balancing redox equations, calculation of the equilibrium constant of redox reactions, calculating titration curves, detection of end point, visual indicators and potentiometric end point detection. Quantitative applications - adjusting the analyte's oxidation state, selecting and standardizing a titrant. Inorganic analysis - chlorine residuals, dissolved oxygen in water, water in non-aqueous solvents. Organic analysis - chemical oxygen demand (COD) in natural and waste waters, titrations of mercaptans and ascorbic acid with I_3^- and titration of organic compounds using periodate.

[16 HOURS]

References:

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch, 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th edition, 2001, John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993, Prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003, Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
6. Principles and Practice of Analytical Chemistry, F.W. Fifield and Kealey, 3rd edition, 2000, Blackwell Sci., Ltd. Malden, USA.
7. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.

CHI HCT: 1.2. INORGANIC CHEMISTRY-I**UNIT – I**

Molecular symmetry and group theory: Symmetry elements and symmetry operations. Concept of a group, definition of a point group. Classification of molecules into point groups. Subgroups. Schoenflies and Hermann-Mauguin symbols for point groups. Multiplication tables (C_n , C_{2v} and C_{3v}). Matrix notation for the symmetry elements. Classes and similarity transformation.

Representation of groups: The Great Orthogonality theorem and its consequences. Character tables (C_s , C_i , C_2 , C_{2v} , C_{2h} and C_{3v}).

Applications of group theory: Group theory and hybrid orbital. Group theory to Crystal field theory and Molecular orbital theory (octahedral and tetrahedral complexes). Determining the symmetry groups of normal modes (both linear and non-linear molecules).

[16 HOURS]

UNIT – II

Structures and energetics of inorganic molecules: Introduction, Energetics of hybridization. VSEPR model for explaining structure of AB, AB₂E, AB₃E, AB₂E₂, ABE₃, AB₂E₃, AB₄E₂, AB₅E and AB₆ molecules. M.O. treatment of homonuclear and heteronuclear diatomic molecules. M.O. treatment involving delocalized π -bonding (CO₃²⁻, NO₃⁻, NO₂⁻, CO₂ and N₃⁻).

Non-aqueous solvents: Classification of solvents, Properties of solvents (dielectric constant, donor and acceptor properties) protic solvents (anhydrous H₂SO₄, HF and glacial acetic acid) aprotic solvents (liquid SO₂, BrF₃ and N₂O₄). Solutions of metals in liquid ammonia. Super acids.

Electron deficient compounds: Higher boranes, polyhedral boranes (preparations, properties, structure and bonding). Wade's rules, carboranes and metallocarboranes.

Lanthanides & Actinides: Spectral & magnetic properties. Use of lanthanide compounds as shift reagents.

[16 HOURS]

UNIT – III

Fundamental concepts: Introduction, Classification of organometallic compounds by bond type, nomenclature, the effective atomic number rule, complexes that disobey the EAN rule, common reactions used in complex formation.

Organometallics of transition metals: Preparation, bonding and structures of nickel, cobalt, iron and manganese carbonyls. Preparation and structures of metal nitrosyls in organometallics.

Ferrocene and ruthenocene: Preparation, structure and bonding.

Complexes containing alkene, alkyne, arene and allyl ligands: preparation, structure and bonding. The isolobal principles.

[16 HOURS]

References:

1. Symmetry and spectroscopy of molecules, 2nd Ed. Veera Reddy, New Age International Publication (2009).
2. Group Theory and its Chemical Applications, P.K. Bhattacharya, Himalaya Publishing House (1986).
3. Chemical Applications of Group Theory, 3rd Ed., F.A. Cotton, Wiley, New York (1990).
4. Inorganic Chemistry, 3rd edition. James E. Huheey, Harper and Row Publishers (1983).
5. Inorganic Chemistry, 3rd edition. G.L. Miessler and D.A. Tarr, Pearson Education (2004).
6. Inorganic Chemistry, 4th edition. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Oxford University Press (2004).

7. Inorganic Chemistry, 2nd edition. C.E. Housecroft and A.G. Sharpe, Pearson Education Ltd. (2005).
8. Basic Organometallic Chemistry - B.D. Gupta and A.J. Elias, Universities Press (2010).

CHO HCT: 1.3. STEREOCHEMISTRY; MOLECULAR REARRANGEMENTS AND HETEROCYCLIC CHEMISTRY

UNIT – I

Stereoisomerism: Projection formulae [Fly wedge, Fischer, Newman and Saw horse], enantiomers, diastereoisomers, configurational notations of simple molecules, *DL* and *RS* configurational notations.

Stereoselectivity: Stereoselective reactions, diastereoselective reactions, stereospecific reactions, regioselective and regiospecific reactions, enantioselective and enantiospecific reactions.

Optical isomerism: Conditions for optical isomerism, Elements of symmetry – plane of symmetry, centre of symmetry, alternating axis of symmetry (rotation-reflection symmetry); optical isomerism due to chiral centers and molecular dissymmetry, allenes and biphenyls, criteria for optical purity.

Geometrical isomerism: Due to C=C, C=N and N=N bonds, E, Z conventions, determination of configuration by physical and chemical methods.

Conformational isomerism: Elementary account of conformational equilibria of ethane, butane and cyclohexane. Conformation of cyclic compounds such as cyclopentane, cyclohexane, cyclohexanone derivatives and decalins. Conformational analysis of 1,2, 1,3, and 1,4-disubstituted cyclohexane derivatives and *D*-Glucose, Effect of conformation on the course/ rate of reactions.

[16 HOURS]

UNIT – II

Molecular rearrangements: Introduction

Carbon to carbon migration: Pinacol-pinacolone, Wagner-Meerwein, Benzidine, Demjanov, benzylic acid, Favorskii, Arndt-Eistert synthesis, Fries rearrangement, Steven's rearrangement, dienophile rearrangement.

Carbon to nitrogen migration: Hofmann, Curtius, Lossen, Schmidt and Beckmann rearrangements.

Miscellaneous rearrangements: Sommelet-Hauser, Wittig, Smiles, Neber, Japp-Klingemann rearrangement, Meisenheimer rearrangements, Bayer-Villegier rearrangement, Allylic rearrangements.

[16 HOURS]

UNIT – III

Heterocyclic chemistry: Nomenclature of heterocyclic systems

Structure, reactivity, synthesis and reactions of indole, pyridine, benzofuran, quinoline, isoquinoline, pyrazole, imidazole, pyrone, coumarin, chromones, pyrimidines and purines. Synthesis and synthetic applications of azirines and aziridines, isoxazole and azepine.

[16 HOURS]

References:

1. H. Pine, Hendrickson, Cram and Hammond, Organic Chemistry, Mc Graw Hill, New York, 1987.
2. Organic Chemistry by Morrison & Boyd.
3. I.L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
4. E.L. Eliel and S.H. Wilen, Stereochemistry of Organic Compounds, John Wiley and Sons, New York. 1994.
5. Introduction to Stereochemistry by K. Mislow.
6. Basic Principles of Organic Chemistry by Roberts & Caserio
7. N.S. Issacs, Reactive Intermediates in Organic Chemistry, John Wiley and Sons, New York. 1974.
8. R.K. Bansal, Organic Reaction Mechanism, Wiley Eastern Limited, New Delhi, 1993.
9. J. March, Advanced Organic Chemistry, Wiley Interscience, 1994.
10. E.S. Gould, Mechanism and Structure in Organic Chemistry, Halt, Rinhart & Winston, New York, 964.
11. A Guide Book to Mechanism in Organic Chemistry by Petersykes
12. Stereochemistry and Mechanism through Solved Problems by P.S. Kalsi.
13. Text book of Organic Chemistry by P.S. Kalsi.
14. F.A. Carey and Sundberg, Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York, 1990.
15. D. Nasipuri, Stereochemistry of Organic Compounds, 2nd edition, Wiley Eastern Limited, New Delhi, 1991.
16. S.K. Ghosh, Advanced General Organic Chemistry, Book and Alleied (P) Ltd, 1998.
17. Heterocyclic Chemistry – Joule & Smith
18. Heterocyclic Chemistry – Achaeson
19. Basic Principles of Heterocyclic Chemistry – L.A. Pacquette
20. Comprehensive Heterocyclic Chemistry – Kartritzky series, Pergamon Press, New York, 1984.

CHP HCT: 1.4. PHYSICAL CHEMISTRY - I

UNIT – I

Concepts of entropy and free energy: Second law of thermodynamics, definition of entropy, entropy of phase transition, entropy change during spontaneous process. Helmholtz and Gibbs free energies, Maxwell relations, Variation of free energy with temperature and pressure. Third law of thermodynamics, Nernst heat theorem & its applications, numericals based on entropy and free energy changes.

Partial molar properties: Partial molar quantities, Partial molar Gibbs function, Partial molar volume and its determination by intercept method and density measurements. Chemical potential and its significance. Variation of chemical potential with temperature and pressure. Formulation of the Gibbs Duhem equation. Derivation of Duhem-Margules equation.

Fugacity: Determination of fugacity of gases. Variation of fugacity with temperature and pressure. Activity and activity coefficients. Variation of activity with temperature and pressure. Determination of activity coefficients by vapour pressure, depression in freezing points and solubility measurements by electrical methods.

Statistical thermodynamics: Different types of ensembles, ensemble averaging, distribution law (Boltzmann statistics), partition function and thermodynamic parameters; relation between molecular and molar partition functions, translational partition function, rotational partition function for linear and non-linear molecules.

[16 HOURS]

UNIT – II

Chemical Kinetics: Introduction

Kinetic equations for complex reactions: Chain, parallel, opposing and consecutive reactions.

Kinetics of fast reactions: Flow methods, continuous and stopped flow methods, Relaxation methods (T-jump and P-jump methods), flash photolysis, pulse and shock tube methods.

Experimental verification: Theory of reaction rates, Temperature effect on reaction rates, Rate constant for simple bimolecular reactions, Collision theory, activated complex theory.

Reactions in solutions: Ionic reactions-salt and solvent effects. Oscillatory reactions: oxidation of malonic acid.

Reaction in surfaces: Langmuir adsorption isotherm; kinetics of surface catalyzed unimolecular & bimolecular reactions, applications in ammonia synthesis.

Kinetic Isotope Effect: Theory of kinetic isotope effect - normal and inverse isotope effect, primary isotope effect, secondary isotope effect, solvent isotope effect.

Linear free energy relationship: Hammett equation, Taft equation. Isokinetic relationship and significance of isokinetic temperature.

Enzyme kinetics: Effect of substrate concentration (Michaelis Menton equation), Effect of pH , effect of catalysts and inhibitors, effect of temperature.

[16 HOURS]

UNIT – III

Electrochemistry: Arrhenius theory of strong and weak electrolytes and its limitations. Factor effecting conductance, Debye-Huckel-Onsager equation of conductivity and its validity. Walden's rule and its application. Debye-Huckel theory - concept of Ionic strength, Debye-Huckel limiting law (DHL), its modification for appreciable concentrations. A brief survey of Helmholtz-Perrin, Guoy-Chapman and Stern electrical double layer (no derivation). Determination of transference number by moving boundary and Hittorf's methods. True and apparent transference numbers (TrN). Abnormal TrN , effect of temperature on TrN . Liquid junction potential-determination and minimization.

Energetics of cell reactions: Effect of temperature, pressure and concentration on energetics of cell reactions (calculation of ΔG , ΔH and ΔS). Electrochemical energy sources – batteries, classification, characteristics, primary, secondary and lithium batteries.

[16 HOURS]

References:

1. Thermodynamics for Chemists by S. Glasstone, Affiliated East-West Press, New Delhi, (1965).
2. Chemical Thermodynamics by I.M. Klotz, W.A. Benzamin Inc. New York, Amsterdam (1964).
3. Basic Physical Chemistry by W.J. Moore, Prentice Hall of India Pvt. Ltd., New Delhi (1986).
4. Text Book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2nd edition (1974).
5. Theoretical Chemistry by S. Glasstone.
6. Elementary Statistical Thermodynamics by N.D. Smith Plenum Press, NY (1982).

7. Elements of Physical Chemistry by Lewis and Glasstone.
8. Physical Chemistry by P.W. Atkins, ELBS, 4th edition, Oxford University Press (1990)
9. Chemical Kinetics by K.J. Laidler.
10. Chemical Kinetics by Frost and Pearson.
11. Kinetics and Mechanism of Chemical Transformation by J. Rajaram and J.C. Kuriacose.
12. Chemical Kinetics by L.K. Jain.
13. Chemical Kinetics by Benson.
14. Kinetics in Analytical Chemistry by H.B. Mark and G.A. Rechnitz, Wiley Interscience Publishers, John Wiley and Sons, New York.
15. Introduction to Electrochemistry by S. Glasstone.
16. Advances in Photochemistry - Rohatgi Mukherjee.
17. Principle and Applications of Photochemistry by R.P. Wayne, Elsevier, New York, (1970).

PRACTICALS – HARD CORE

CHA HCP: 1.5. ANALYTICAL CHEMISTRY PRACTICALS

[128 HOURS]

PART – I

1. Determination of total acidity of vinegar and wines by acid-base titration.
2. Determination of purity of a commercial boric acid sample, and Na_2CO_3 content of washing soda.
3. Analysis of chromate-dichromate mixture by acid-base titration.
4. Determination of replaceable hydrogen and relative molecular mass of a weak organic acid by titration with NaOH.
5. Determination of ephedrine and aspirin in their tablet preparations by residual acid-base titrimetry.
6. Determination of purity of aniline and assay of chlorpromazine tablets by non-aqueous acid-base titration.
7. Periodate determination of ethylene glycol and glycerol (Malprade reaction).
8. Determination of carbonate and bicarbonate in a mixture by *pH*-metric titration and comparison with visual acid-base titration.
9. Determination of purity of a commercial sample of mercuric oxide by acid-base titration.
10. Determination of benzoic acid in food products by titration with methanolic KOH in chloroform medium using thymol blue as indicator.
11. Determination of the *pH* of hair shampoos and *pH* determination of an unknown soda ash.
12. Analysis of water/ waste water for acidity by visual, *pH* metric and conductometric titrations.
13. Analysis of water/ waste water for alkalinity by visual, *pH* metric and conductometric titrations.
14. Determination of carbonate and hydroxide-analysis of a commercial washing soda by visual and *pH*-titrimetry.
15. Determination of ammonia in house-hold cleaners by visual and conductometric titration.
16. Potentiometric determination of the equivalent weight and K_a for a pure unknown weak acid.
17. Spectrophotometric determination of creatinine and phosphorus in urine.
18. Flame emission spectrometric determination of sodium and potassium in river/ lake water.
19. Spectrophotometric determination of *pK_a* of an acid-base indicator.

PART – II

1. Determination of percentage of chloride in a sample by precipitation titration - Mohr, Volhard and Fajan's methods.
2. Determination of silver in an alloy and Na_2CO_3 in soda ash by Volhard method.
3. Mercurimetric determination of blood or urinary chloride.
4. Determination of total hardness, calcium and magnesium hardness and carbonate and bicarbonate hardness of water by complexation titration using EDTA.
5. Determination of calcium in calcium gluconate/ calcium carbonate tablets/ injections and of calcium in milk powder by EDTA titration.
6. Analysis of commercial hypochlorite and peroxide solution by iodometric titration.
7. Determination of copper in an ore/ an alloy by iodometry and tin in stibnite by iodimetry.
8. Determination of ascorbic acid in vitamin C tablets by titrations with KBrO_3 and of vitamin C in citrus fruit juice by iodimetric titration.
9. Determination of iron in razor blade by visual and potentiometric titration using sodium metavanadate.
10. Determination of iron in pharmaceuticals by visual and potentiometric titration using cerium(IV) sulphate.
11. Determination of nickel in steel by synergic extraction and boron in river water/ sewage using ferroin.
12. Determination of total cation concentration of tap water by ion-exchange chromatography.
13. Determination of magnesium in milk of magnesium tablets by ion-exchange chromatography.
14. Cation exchange chromatographic separation of cadmium and zinc and their estimation by EDTA titration.
15. Gas chromatographic determination of ethanol in beverages.
16. Determination of aspirin, phenacetin and caffeine in a mixture by HPLC.
17. Solvent extraction of zinc and its spectrophotometric determination.
18. Anion exchange chromatographic separation of zinc and magnesium followed by EDTA titration of the metals.
19. Separation and determination of chloride and bromide on an anion exchanger.
20. Thin layer chromatographic separation of amino acids.

References:

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th edition, 2001 John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993, Prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003, Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
6. Practical Clinical biochemistry methods and interpretations, R. Chawla, J.P. Bothers Medical Publishers (P) Ltd., 1995.
7. Laboratory manual in biochemistry, J. Jayaraman, New Age International Publishers, New Delhi, 1981.
8. Practical Clinical Biochemistry by Harold Varley and Arnold.Heinmann, 4th edition.

CHI HCP: 1.6. INORGANIC CHEMISTRY PRACTICALS

[128 HOURS]

PART – I

1. Determination of iron in haematite using cerium(IV) solution (0.02M) as the titrant, and gravimetric estimation of insoluble residue.
2. Estimation of calcium and magnesium carbonates in dolomite using EDTA titration, and gravimetric analysis of insoluble residue.
3. Determination of manganese dioxide in pyrolusite using permanganate titration.
4. Quantitative analysis of copper-nickel in alloy/ mixture:
 - i. Copper volumetrically using KIO_3 .
 - ii. Nickel gravimetrically using DMG
5. Determination of lead and tin in a mixture: Analysis of solder using EDTA titration.
6. Quantitative analysis of chloride and iodide in a mixture:
 - i. Iodide volumetrically using KIO_3
 - ii. Total halide gravimetrically
7. Gravimetric analysis of molybdenum with 8-hydroxyquinoline.

8. Micro-titrimetric estimation of :
 - a) Iron using cerium(IV)
 - b) Calcium and magnesium using EDTA
9. Quantitative estimation of copper(II), calcium(II) and chloride in a mixture.
10. Circular paper chromatographic separation of: (Demonstration)
 - a. Iron and nickel
 - b. Copper and nickel

PART – II

Semimicro qualitative analysis of mixtures containing **TWO** anions and **TWO** cations (excluding sodium, potassium and ammonium cations) and **ONE** of the following less common cations: W, Mo, Ce, Th, Ti, Zr, V, U and Li.

References:

1. Vogel's Text Book of Quantitative Chemical Analysis – 5th edition, J. Basset, R.C. Denney, G.H. Jeffery and J. Mendhom.
2. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel, 3rd edition.
3. Spectrophotometric Determination of Elements by Z. Marczenko.
4. Vogel's Qualitative Inorganic Analysis – Svelha.
5. Macro and Semimicro Inorganic Qualitative Analysis by A.I. Vogel.
6. Semimicro Qualitative Analysis by F.J. Welcher and R.B. Halin.
7. Quantitative Chemical Analysis by Daniel C. Harris, 7th edition, (2006).

CHO HCP: 1.7. ORGANIC CHEMISTRY PRACTICALS

[128 HOURS]

PART – I

1. Preparation of *p*-nitro aniline from acetanilide.
2. Preparation of n-butyl bromide from n-butanol.
3. Preparation of *p*-nitroiodobenzene from paranitroaniline.
4. Preparation of aniline from nitrobenzene.
5. Preparation of β -D-Glucose penta acetate.
6. Preparation of phenoxy acetic acid.
7. Preparation of cyclohexanone from cyclohexanol.
8. Preparation of chalcone.

9. Preparation of *S*-benzylthiuronium chloride.
10. Condensation of anthracene and maleic anhydride (Diels-Alder reaction).
11. Preparation of *m*-nitrobenzoic acid from methyl benzoate.

PART – II

Qualitative analysis: Separation of binary mixtures, identification of functional groups and preparation of suitable solid derivatives.

CHP HCP: 1.8. PHYSICAL CHEMISTRY PRACTICALS

[128 HOURS]

PART – I (Non-instrumental)

1. Study of kinetics of hydrolysis of an ester using HCl/ H₂SO₄ at two different temperature, determination of rate constants and energy of activation.
2. Kinetics of the Iodine-hydrogen peroxide clock reaction.
3. Determination of activation energy for the bromide-bromate reaction
4. Determination of heat of solution of benzoic acid by variable temperature method (graphical method).
5. Determination of partial molar volume of NaCl-H₂O system.
6. Determination of critical solution temperature of phenol-water system.
7. Binary analysis of two miscible liquids by viscometric method (Ethanol & Water)
8. Determination of molecular weight of polymer by viscosity method.

PART – II (Instrumental)

1. Conductometric titration of a mixture of HCl and CH₃COOH against NaOH.
2. Conductometric titration of orthophosphoric acid /formic acid/ oxalic acid against NaOH and NH₄OH.
3. Determination of PI of glycine by potentiometric method.
4. Determination of dissociation constant of a weak acid by potentiometric method.
5. pH titration of (a) polybasic acid(H₃PO₄), (b) (CH₃COOH+HCl) and (c) CuSO₄ vs NaOH and determination of k_a .
6. To obtain the absorption spectra of coloured complexes, verification of Beer's law and estimation of Ni⁺² ions from [Ni(NH₃)₆]²⁺ by spectrophotometry.
7. Analysis of binary mixture (Glycerol and Water) by the measurement of refractive index.

8. Study the kinetics of reaction between CAT and indigocarmine spectrophotometrically and determination of rate constant.

References:

1. Practical Physical Chemistry – A.J. Findlay.
2. Experimental Physical Chemistry – F. Daniels *et al.*
3. Selected Experiments in Physical Chemistry – Latham.
4. Experiments in Physical Chemistry – James and Prichard.
5. Experiments in Physical Chemistry – Shoemaker.
6. Advanced Physico-Chemical Experiments – J. Rose.
7. Practical Physical Chemistry – S.R. Palit.
8. Experiments in Physical Chemistry – Yadav, Geol Publishing House.
9. Experiments in Physical Chemistry – Palmer.
10. Experiments in Chemistry – D.V. Jahagirdar, Himalaya Publishing House, Bombay, (1994).
11. Experimental Physical Chemistry – R.C. Das. and B. Behera, Tata Mc Graw Hill.

THEORY – SOFT CORE

CHA SCT 1.1: APPLIED ANALYSIS I

UNIT – I

Air pollution, analysis and control: Historical overview - global implications of air pollution, sources of pollutants, classification of pollutants. Sources and effects of particulates, carbon monoxide, sulphur oxides, nitrogen oxides, hydrocarbons and photochemical oxidants on human health, vegetation and materials. Standards for air pollutants.

Air quality monitoring: Sampling methods and devices for particulates and gaseous pollutants. SO₂: ambient air measurements and stack gas measurements - Turbidimetric, colorimetric, conductometric and coulometric methods, NO_x: Griess-Ilosvay and Jacobs-Hockheiser colorimetric methods, Hydrocarbons: total and individual hydrocarbons by gas chromatography. Oxidants and ozone: colorimetric, titrimetric and chemiluminescence methods.

Control devices for particulates: Gravitational settlers, centrifugal collectors, wet collectors, electrostatic precipitation and fabric filtration.

Control devices for gaseous pollutants: adsorption, absorption, condensation and combustion processes. Automotive emission control-catalytic converters.

Water pollution and analysis: Water resources, origin of wastewater, types of water pollutants; their sources and effects, chemical analysis for water pollution control - objectives of analysis, parameters of analysis, sample collection and preservation. Environmental and public health significance and measurement of colour, turbidity, total solids, acidity, alkalinity, hardness, chloride, residual chlorine, chlorine demand, sulphate, fluoride, phosphates and different forms of nitrogen in natural and waste/ polluted waters, heavy metal pollution - public health significance of Pb, Cd, , Hg, and As, general survey of the instrumental techniques for the analysis of heavy metals in aquatic systems, organic loadings - significance and measurement of DO, BOD, COD, TOD, and TOC.

[16 HOURS]

UNIT – II

Food analysis: Objectives of food analysis. Sampling procedures. Detection and determination of sugars and starch. Methods for protein determination. Oils and fats and their analysis - iodine value, saponification value and acid value. Rancidity - detection and determination (peroxide number). Tests for common edible oils. Analysis of foods for minerals - phosphorus, sodium, potassium and calcium. General methods for the determination of moisture, crude fibre and ash contents of food. Analysis of milk for fat and added water. Non-alcoholic beverages - determination of chicory and caffeine in coffee; caffeine and tannin in tea. Alcoholic beverages - methanol in alcoholic drinks and chloral hydrate in toddy. Food additives - chemical, preservatives - inorganic preservatives - sulphur dioxide and sulphites, their detection and determination. Organic preservatives - benzoic acid and benzoates, their detection and determination. Flavouring agents - detection and determination of vanilla and vanillin. Coloring matters in foods - classification, certified colors, detection of water soluble dyes, color in citrus fruits, beet dye in tomato products, mineral color. Pesticide residues in foods - determination of chlorinated organic pesticides. Control food quality - codex alimentarius, Indian standards.

Drugs and pharmaceutical analysis: Importance of quality control; drugs and pharmaceuticals. Sources of impurities in pharmaceutical chemicals. Analytical quality control in finished/ final products. Common methods of assay. Analysis of common drugs; Analgesics - aspirin, paracetamol; Anthelmintics - mebendazole; Antiallergies - chlorpheniramine maleate; Antibiotics - penicillin, chloromycetin; Anti-inflammatory agents - oxyphenbutazone; Antimalarials - primaquine phosphate; Antituberculosists - INH; Narcotics - nicotine, morphine; Expectorants - Benadryl; Sedative - diazepam; Vitamins - A, C, B1, B2, B6, niacin and folic acid.

[16 HOURS]

References:

1. Standard Methods of Chemical Analysis, A.J. Weleher (Part B), Robert E. Krieger Publishing Co. USA, 1975.
2. Environmental Chemistry, S.E. Manahan Willard grant press, London, 1983.
3. Environmental Chemical Analysis, Iain L Marr and Malcolm S. Cresser, Blackie and Son Ltd., London, 1983.
4. Chemistry for Environmental Engineering, Chair N. Sawyer and Perry L.M Canty, Mcgraw Hill Book, Co., New York, 1975.
5. The Air Pollution Hand Book, Richard Mabey, Penguin, 1978.
6. The Pollution Hand Book, Richard Mabey, Ponguin 1978.
7. Soil Chemical Analysis, M.L. Jackson, Prentice Hall of India Pvt, Ltd., New Delhi, 1973.
8. Experiments in Environmental Chemistry, P.D. Vowler and D.W. Counel, Pergamon press, Oxford 1980.
9. Manual Soil Laboratory Testing, vol I, K.H. Head, Pentech Press, London 1980.
10. A Text Book of Environmental Chemistry and Pollution Control, S.S. Dara, S. Chand and co. Ltd. New Delhi 2004.
11. Air pollution Vol II edition by A.C. Stern, Academic Press New York, 1968.
12. Instrumental Methods for Automatic Air Monitoring Systems in Air Pollution Control, Part-III edition by W. Stranss, John-Wiley and Sons, New York, 1978.
13. Analysis of Air pollutants, P.O. Warner, John Wiley and Sons, New York, 1976.
14. The Chemical Analysis Air pollutants, Interscience, New York, 1960.
15. The Analysis of Air Pollutants, W. Liethe, Ann Arbor Science Pub. Inc. Michigan 1970.
16. Environmental Chemistry, A. K. De.
17. Food Analysis, A.G. Woodman, McGraw Hill. 1971.
18. Chemical Analysis of Foods, H.E. Cox and Pearson.
19. Analysis of Foods and Food Products, J.B. Jacob.
20. A First Course in Food Analysis, A.Y. Sathe, New Age Internationals (P) Ltd., Publishers, Bangalore, 1999.
21. Analytical Agricultural Chemistry, S.L. Chopra and J.S. Kanwar, Kalyani Publishers, New Delhi, 1999.
22. Pharmaceutical Analysis, (Ed). T. Higuchi and E.B. Hanssen, John Wiley and Sons, New York, 1997.
23. Pharmaceutical Analysis - Modern Methods, Part A and B, (Ed). James W. Hunson.
24. Quantitative Analysis of Drugs in Pharmaceutical Formulations, P. D. Sethi, 3rd edition. CBS Publishers and Distributors, New Delhi, 1997.

CHI SCT 1.2: FRONTIERS IN INORGANIC CHEMISTRY

UNIT – I

Materials chemistry

General principles-Defects, nonstoichiometric compounds and solid solutions, atom and ion diffusion, solid electrolytes. Synthesis of materials-The formation of extended structures, chemical deposition.

Metal oxides, nitrides and fluorides: Monoxides of the 3d metals, higher oxides and complex oxides, oxide glasses, nitrides and fluorides.

Chalcogenides, intercalation chemistry and metal rich phases: Layered MS₂ compounds and intercalation, Chevrel phases.

Framework structures: Structures based on tetrahedral oxoanions, structures based on octahedral and tetrahedral.

Inorganic pigments: Coloured pigments, white and black inorganic materials.

Molecular materials and fullerenes: Fullerenes, Molecular material chemistry.

Silicates: Structure, classification - silicates with discrete anions, silicates containing chain anion, silicates with layer structure, silicones with three dimensional net work and applications.

[16 HOURS]

UNIT – II

Nanomaterials, nanoscience and nanotechnology

Fundamentals-Terminology and history, novel optical properties of nanomaterials.

Characterization and fabrication: Characterization methods. Top-down and bottom-up fabrication. Solution based synthesis of nanoparticles. Vapour-phase synthesis of nanoparticles. Synthesis using frameworks, supports and substrates.

Artificially layered materials: Quantum wells and multiple quantum wells. Solid state superlattices. Artificially layered crystal structures.

Self-assembled nanostructures: Self-assembly and bottom-up fabrication. Supramolecular chemistry and morphosynthesis. Dimensional control in nanostructures.

Bioinorganic nanomaterials: DNA and nanomaterials. Natural and artificial nanomaterials-Biomimetics. Bionanocomposites.

Inorganic-organic nanocomposites: Uses and design strategies. Polymer nanocomposites.

[16 HOURS]

References:

1. Inorganic Chemistry, 4th edition. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Oxford University Press (2006).

- Inorganic Chemistry Principles of Structure and Reactivity: James E. Huheey, Ellen A. Keiter, Richard L. Keiter, Okhil K. Medhi, Delhi University, New Delhi (2006)
- Chemistry of the Elements – N.N. Greenwood and A. Earnshaw, Pergamon Press (1985).
- Industrial Inorganic Chemistry – 2nd edition. K.H. Buchel, H.H. Moretto and P. Woditsh, Wiley - VCH (2000).
- Basic Inorganic Chemistry – 3rd edition. F.A. Cotton, G. Wilkinson and P.L. Gaus, John Wiley and Sons (2002).
6. Inorganic Chemistry, 3rd edition. James E. Huheey, Harper and Row Publishers (1983).
- Inorganic Chemistry, 3rd edition. G.L. Miessler and D.A. Tarr, Pearson Education (2004).
- Inorganic Chemistry, 2nd edition. C.E. Housecroft and A.G. Sharpe, Pearson Education.

CHO SCT 1.3: REACTION MECHANISMS

UNIT – I

Structure and reactivity: Brief discussion on effects of hydrogen bonding, resonance, inductive and hyperconjugation on strengths of acids and bases.

Methods of determining organic reaction mechanism: Thermodynamic and kinetic requirements for reactions, kinetic and thermodynamic control. Hammonds postulates and Curtin-Hammett principle.

Identification of products. Formation, structure, stability, detection and reactions of carbocations (classical and non-classical), carbanions, free radicals, carbenes, nitrenes, nitrile oxides, nitrile imines, nitrile ylides and arynes. Determination of reaction intermediates, isotope labeling and effects of cross over experiments. Kinetic and stereochemical evidence, solvent effect. Linear free energy relationship-Hammett equation and Taft treatment.

[16 HOURS]

UNIT – II

Basics of organic reactions: Meaning and importance of reaction mechanism, classification and examples for each class.

Aliphatic substitution reactions:

Nucleophilic substitution reactions: Kinetics, mechanism and stereochemical factors affecting the rate of S_N^1 , S_N^2 , S_N^i , S_N^1 , S_N^2 and S_N^i reactions, Neighbouring group participation.

Electrophilic substitution reactions: S_E^1 and S_E^2 reactions

Aromatic substitution reactions:

Nucleophilic substitution reactions: S_N^1 , S_N^2 and benzyne mechanism, Bucherer reaction.

Electrophilic substitution reactions: Mechanism of Friedel-Crafts alkylation and acylation, Mannich reaction, chloromethylation, Vilsmeier-Haack reaction.

Mechanism of hydrolysis of carboxylic acid derivatives: Hydrolysis of esters, amides and acid chlorides.

Elimination reactions: Mechanism and stereochemistry of eliminations - E_1 , E_2 , E_{1cB} . *cis* elimination, Hofmann and Saytzeff eliminations, competition between elimination and substitution, decarboxylation reactions. Chugaev reaction.

[16 HOURS]

References:

1. Organic Chemistry by Morrison and Boyd.
2. H. Pine, Hendrickson, Cram and Hammond, Organic Chemistry, Mc Graw Hill, New York, 1987.
3. I.L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
4. E.L. Eliel and S.H. Wilen, Stereochemistry of Organic Compounds, John Wiley and Sons, New York. 1994.
5. Basic Principles of Organic Chemistry by Roberts & Caserio
6. N.S. Issacs, Reactive Intermediates in Organic Chemistry, John Wiley and Sons, New York. 1974.
7. R.K. Bansal, Organic Reaction Mechanism, Wiley Eastern Limited, New Delhi, 1993.
8. J. March, Advanced Organic Chemistry, Wiley Interscience, 1994.
9. A Guide Book to Mechanism in Organic Chemistry by Petersykes
10. Stereochemistry and Mechanism through Solved Problems by P.S. Kalsi.
11. Text book of Organic Chemistry by P.S. Kalsi.
12. F.A. Carey and Sundberg, Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York, 1990.
13. S.K. Ghosh, Advanced General Organic Chemistry, Book and Alleied (P) Ltd, 1998.
14. Organic chemistry, Gram Solomons.

CHP SCT 1.4: SOLID STATE CHEMISTRY AND CHEMISTRY OF NANOMATERIALS

UNIT – I

Solid state chemistry: Types of imperfections, classification of imperfections, point defects, Schottky defects, Frenkel defects, disordered crystals, line defects, dislocation types, plane defects, small-angle and large-angle boundaries, stacking faults, crystal growth and twinning.

X-ray crystallography: law of interfacial angles, laws of symmetry, Miller indices, Bragg equation (no derivation), Experimental methods – powder and rotating crystal methods, indexing of powder and rotating crystal photographs. Atomic scattering factor, structure factor, Fourier synthesis and electron density diagrams. Electron diffraction of gases, experimental technique, Scattering-Intensity curves, Wierl equation (no derivation), Radial distribution method determination of bond lengths and bond angles. Heat capacity of solids: Einstein and Debye equations (with derivation).

[16 HOURS]

UNIT – II

Semiconductors: Band theory, energy bands, intrinsic and extrinsic semiconductors. Conductivity: electrons and holes, temperature dependence on conductivity, Optical properties: absorption spectrum, photoconductivity, photovoltaic effect and luminescence. Junction properties: metal-metal junctions, metal-semiconductor junctions, p-n junctions, transistors, industrial applications of semiconductors: Mixed oxides, spinels and other magnetic materials.

Superconductors: Meissner effect, type I and II super conductors, isotope effect, basic concepts of BCS theory, manifestations of the energy gap, Josephson devices.

Chemistry of nanomaterials: Nano particles. Synthesis - Laser ablation, chemical vapour transportor (CVT) and sol-gel methods. Metal oxides nanoparticles with supercritical water and precursor method. Synthesis of metal oxides and its composite nanoparticles by solvothermal and hydrothermal methods. Carbon nanotube, carbon nanowires and its composites. Applications of nanomaterials in renewable energy. Inorganic and organic nanoporous aerogels.

[16 HOURS]

References:

1. Introduction to Solids, Azaroff.
2. Solid State Chemistry and its Applications, Anthony R. West.
3. Basic Solid State Chemistry, 2nd edition, Anthony R. West.
4. Solid State Chemistry: An Introduction, 3rd edition, Lesley E. Smart and Elaine A. Moore.

5. Introduction to Solid State Physics - C. Kittel, 5th edition, Wiley Eastern Ltd.
6. New Directions in Solid State Chemistry - C.N.R. Rao and J. Gopalakrishna, Cambridge University Press, Cambridge (1999).
7. Advances in Technologically Important Crystals - Binay Kumar, R.P. Tandon, Mcmillan.
8. Hand Book of Nanotechnology, Bharat Bhushan, Springer Publisher.
9. Nanotechnology, Richard Booker and Earl Boysen, Wiley.
10. Nanomaterials, A.K. Bandopadhyay, New Age International, 2nd edition.
11. Nanotechnology - Importance and Applications, M. H. Fulekar, Ink International publisher.

SECOND SEMESTER

THEORY – HARD CORE

CHA HCT: 2.1. SEPARATION TECHNIQUES

UNIT – I

Solvent extraction: Theory - Nernst partition law, efficiency and selectivity of extraction.

Extraction systems: Extraction of covalent neutral molecules, extraction of uncharged metal chelates and synergic extraction, extraction of ion-association complexes - non chelated complexes, chelated complexes and oxonium systems. Use of salting out agents. Methods of extraction - batch and continuous extractions. applications.

Solid Phase Extraction (SPE): Principles, apparatus and instrumentation. Solid phase sorbents, extraction formats - Automated solid phase extraction. Solid phase micro extraction (SPME). Applications of SPE and SPME.

Chromatography: Definition, principles and mechanism of separation, classification of chromatographic techniques. General descriptions of column chromatography - frontal analysis, displacement analysis and elution analysis. General theory of column chromatography: characterizing a chromatogram - retention time, retention volume and baseline width. Chromatographic resolution, capacity factor, column selectivity. Column efficiency - band broadening - rate theory and plate theory. Peak capacity, non ideal behavior. Optimizing chromatographic separations using capacity factor, column selectivity and column efficiency - Van Deemter equation, and its modern versions, Golay equation and Huber-Knox equations.

[16 HOURS]

UNIT – II

Gas chromatography (GC): Principles, instrumentation - mobile phase, chromatographic columns, stationary phases, sample introduction, temperature control, and detectors for gas chromatography. Quantitative and qualitative applications.

High performance liquid chromatography (HPLC): Principles, instrumentation - columns (analytical and guard columns), stationary phases, mobile phases, choosing a mobile phase, isocratic vs gradient elution, HPLC plumbing, sample introduction. Detectors for HPLC - spectroscopic, electrochemical and others, quantitative applications.

Ion exchange chromatography (IEC): Definitions, requirements for ion-exchange resin, synthesis and types of ion-exchange resins, principle, basic features of ion-exchange reactions, resin-properties-ion-exchange capacity, resin selectivity and factors affecting the selectivity, applications of IEC in preparative, purification and recovery processes. IEC with eluent suppressor columns. Single Column Ion Chromatography.

Size-exclusion chromatography: Theory and principle of size-exclusion chromatography, experimental techniques of gel-filtration chromatography (GFC) and gel-permeation chromatography (GPC), materials for packing - factors governing column efficiency, methodology and applications.

[16 HOURS]

UNIT – III

Thin layer chromatography: Principle, apparatus and methodology, applications, HPTLC

Affinity chromatography: Definitions, separation-mechanism-matrices, matrix activation, role of spacer arms and applications.

Supercritical fluid chromatography (SFC): Properties of supercritical fluids, instrumentation and operating variables, comparison of SFC with other types of chromatography, applications.

Supercritical fluid extraction: Advantages of supercritical fluid extraction, instrumentation, supercritical fluid choice, off-line and on-line extractions, typical applications of supercritical fluid extraction.

Electrophoretic methods - Electrophoresis & Capillary Electrophoresis: Theory - electrophoretic mobility, electroosmotic mobility, electroosmotic flow velocity, total mobility, migration time, efficiency, selectivity and resolution. Instrumentation - capillary tubes, hydrodynamic and electrokinetic methods of sample injection, applying electric field and detectors. Capillary electrophoresis methods - capillary zone electrophoresis, micellar electrokinetic capillary chromatography, capillary gel electrophoresis and capillary electrochromatography.

[16 HOURS]

References:

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th edition, 2001 John Wiley & Sons, Inc. India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993 Prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003 Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
6. Introduction to Instrumental Analysis, Robert. D. Braun, Pharm. Med. Prem. India, 1987.
7. Instrumental Method of Analysis, W.M. Dean and Settle, 7th edition, 1986, CBS Publishers, New Delhi.
8. Instant Notes of Analytical Chemistry, Kealey and Haines, Viva Books Pvt. Ltd., 2002.
9. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.
10. Principles and Practice of Analytical Chemistry, F. W. Fifield and Kealey, 5th edition, 2000, Blackwell Sci., Ltd. Malden, USA.

CHI HCT: 2.2. ADVANCED COORDINATION CHEMISTRY

UNIT – I

Preparation of coordination compounds: Introduction, Preparative methods - simple addition reactions, substitution reactions, oxidation-reduction reactions, thermal dissociation reactions, reactions of coordinated ligands, the trans-effect, other methods.

Stability of coordination compounds: Introduction, trends in stepwise stability constants, factors influencing the stability of metal complexes with reference to the nature of metal ion and ligands, the Irving-William series, chelate effect.

Geometries of metal complexes: coordination numbers 2-10.

Determination of stability constants: Theoretical aspects of determination of stability constants of metal complexes by spectrophotometric, pH metric and polarographic methods.

Crystal field theory: Salient features of CFT, d-orbital splitting in octahedral, tetrahedral, square planar and tetragonal complexes, Jahn-Teller distortions, measurement of $10 Dq$ and factors affecting it. Evidences for metal-ligand covalency.

[16 HOURS]

UNIT – II

Molecular Orbital Theory: Introduction, Principles of Molecular orbital theory, sigma and pi-bonds in MOT. Applications to Ligand field theory. MOT to octahedral, tetrahedral and square planar complexes with and without pi-bonding.

Electronic spectra: Introduction, selection rules and intensities, electronic spectra of octahedral and tetrahedral complexes, Term symbols for d^n ions, Orgel and Tanabe-Sugano diagrams, charge-transfer spectra. Ligand-field transition, Optical rotatory dispersion and Circular dichroism.

Magnetic properties: Origin of magnetism, types of magnetism, Curie law, Curie Weiss law, magnetic susceptibility and its measurements. Spin and orbital contributions to the magnetic moment, the effects of temperature on μ_{eff} , spin-cross over, ferromagnetism, antiferromagnetism and ferrimagnetism.

[16 HOURS]

UNIT - III

Reaction and Mechanisms: Introduction

Substitution reactions - Inert and labile compounds, mechanisms of substitution.

Kinetic consequences of Reaction pathways - Dissociation, interchange and association.

Experimental evidence in octahedral substitution - Dissociation, associative mechanisms, the conjugate base mechanism, the kinetic chelate effect.

Substitution reactions of square-planar complexes - kinetics and stereochemistry of square-planar substitutions, evidence for associative reactions, explanations of the trans effect.

Stereochemistry of reactions- Substitution in trans and its complexes, isomerization of chelate rings.

Electron-transfer processes: Inner-sphere mechanism and outer-sphere mechanism, conditions for high and low oxidation numbers.

Metal-metal bonding: Evidences and factors favoring of M-M bonding, Wade's-Mingo's-Lauher rules, bi, tri, tetra, penta and hexa nuclear metal clusters.

[16 HOURS]

References

1. Physical Inorganic Chemistry - A Coordination Chemistry Approach- S.F.A. Kettle, Spektrum, Oxford, (1996).
2. Inorganic Chemistry - 2nd edition, C.E. Housecroft and A.G. Sharpe, Pearson Education Ltd., (2005).
3. Inorganic Chemistry - 3rd edition, G.L. Miessler and D.A. Tarr, Pearson Education, (2004).
4. Inorganic Chemistry - 2nd edition, D.F. Shriver, P.W. Atkins and C.H. Langford, Oxford University Press, (1994).
5. Inorganic Chemistry- 3rd edition, James E. Huheey, Harper and Row Publishers, (1983).
6. Basic Inorganic Chemistry- 3rd edition, F.A. Cotton, G. Wilkinson and P.L. Gaus, John Wiley and Sons, (2002).

CHO HCT: 2.3. REAGENTS IN ORGANIC SYNTHESIS; PHOTOCHEMISTRY AND PERICYCLIC REACTIONS

UNIT – I

Reductions: Catalytic hydrogenations (homogeneous and heterogeneous) - catalysts, reduction of functional groups, catalytic hydrogen transfer reactions. Wilkinson catalyst. Baker's yeast, LiAlH_4 , NaBH_4 , metal dissolving reactions (Birch reduction). Leukart reaction (reductive amination), diborane, Meerwein-Ponndorf-Verley reduction, Wolf-Kishner reduction, Clemensen reduction, tributyl tinhydride, stannous chloride.

Oxidations: Oxidation with chromium and manganese compounds (CrO_3 , $\text{K}_2\text{Cr}_2\text{O}_7$, PCC, PDC, Sarret reagent, Jones reagent, MnO_2 , KMnO_4), ozone, peroxides and peracids, lead tetra acetate, periodic acid, OsO_4 , SeO_2 , NBS, chloramine-T, Sommelet oxidation, Oppenauer oxidation, Sharpless epoxidation, Woodward and Prevost hydroxylation. Electrochemical Oxidation and reduction of organic compounds, green oxidation agents.

[16 HOURS]

UNIT – II

Reagents in organic synthesis: Use of following reagents in organic synthesis and functional group transformations: Lithium disopropylamide (LDA), Gilmann reagent, dicyclohexyl carbodimide (DCC), dichloro dicyano quinone (DDQ), trialkyl silyl halides, phase transfer catalyst, crown ethers, Fenton's reagent, Ziegler-Natta catalyst, diazomethane, Stark enamine reaction, Phosphorus ylides – Wittig and related reactions, 1,3-dithiane anions - Umpolung

reaction, sulphur ylides – reactions with aldehydes and ketones, Peterson reactions - synthesis of alkenes.

Green Synthesis: Designing of green synthesis, choice of reagents and catalysis. Microwave induced organic synthesis, ionic liquids in organic synthesis, polymer supported reagents and synthesis and the use of ultra sound in organic synthesis.

[16 HOURS]

UNIT – III

Photochemistry and concerted reactions: Introduction, light absorption and electronic transitions, Jablonski diagram, intersystem crossing, energy transfer, sensitizers, quenchers.

Photochemistry of olefins, conjugated dienes, aromatic compounds, ketones, enones, photooxidations, photoreductions, Norrish type I and II reactions, Paterno-Buchi reaction, Barton reaction, Di-pi-rearrangements.

Electrocyclic reactions: Stereochemistry, symmetry and Woodward-Hofmann rules for electrocyclic reactions, FMO theory of electrocyclic reactions, correlation diagram for cyclobutadiene and cyclohexadiene systems.

Cycloaddition reactions: Classification, analysis by FMO and correlation diagram method. **1,3-dipolar cycloadditions:** involving nitrile oxide, nitrile imine, nitrile ylide cycloaddition. Intra and intermolecular 3+2 cycloaddition and their application in organic synthesis. **[4+2]**

cycloaddition reactions: Deils-Alder reaction, hetero Diels-Alder reaction and their applications.

Sigmatropic reactions: Classification, stereochemistry and mechanisms. suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties. [3,3] and [5,5]- sigmatropic rearrangement, Claisen, Cope and aza-Cope rearrangement

[16 HOURS]

References:

1. H. Pine, Hendrickson, Cram and Hammond, Organic Chemistry, Mac Grow Hill, New York, 1987.
2. Organic Chemistry - Morrison and Boyd
3. I.L. Finar, Organic Chemistry, ELBS Longmann, Vol. 1 & II, 1984.
4. J. March, Advanced Organic Chemistry, Wiley Interscience, 1994.
5. E.S. Gould, Mechanism and Structure in Organic Chemistry, Halt, Rinhart & Winston, New York, 1964.

6. F.A. Carey and Sundberg. Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York. 1990.
7. Principles of Organic Synthesis - ROC Norman and Coxon
8. S.K. Ghosh, Advanced General Organic Chemistry, Book and Allied (P) Ltd. 1998.
9. R.K. Kar, Frontier orbital and symmetry controlled Pericyclic reaction.

CHP HCT: 2.4. PHYSICAL CHEMISTRY – II

UNIT – I

Quantum Chemistry: A brief resume of black body radiation, and atomic spectra-Bohr's theory of hydrogen atom. Photoelectric and Compton effects, de-Broglie concept, uncertainty principle, operators (algebra of operators, commutative and non-commutative operators, linear operator, Laplacian operator, Hermitian operator-Hamiltonian operator, turn over rule. Wave equation for stretched strings, Schrodinger wave equation for particles, Eigen values and Eigen functions, postulates of quantum mechanics. Application of Schrodinger equation to a free particle and to a particle trapped in a potential field (one dimension and three dimensions). Degeneracy, Wave equation for H-atom, separation and solution of R, ϕ and θ equations. Application of Schrodinger equation to rigid rotator and harmonic oscillator. Quantum numbers and their characteristics, orbital diagrams.

Approximate methods – Necessity of approximate methods, perturbation method, the theory of perturbation method – first order and second order correction, application to He-atom (first order correction only) – calculation of first ionization potential and binding energy.

[16 HOURS]

UNIT-II

Microwave spectroscopy: Rotation spectra of diatomic Molecules - rigid and non rigid rotator model. Rotational quantum number and the selection rule. Effect of isotopic substitution on rotation spectra. Relative intensities of the spectral lines. Classification of polyatomic molecules based on moment of inertia - Linear, symmetric top, asymmetric top and spherical molecules. Rotation spectra of polyatomic molecules (OCS, CH₃F and BCl₃). Moment of inertia expression for linear tri-atomic molecules. Applications - Principles of determination of Bond length and moment of inertia from rotational spectra. Stark effect in rotation spectra and determination of dipole moments.

Vibration spectroscopy: Vibration of diatomic molecules, vibrational energy curves for simple harmonic oscillator. Effects of anharmonic oscillation. Vibration - rotation spectra of carbon monoxide. Expressions for fundamental and overtone frequencies. Vibration of polyatomic

molecules – The number of degrees of freedom of vibration. Parallel and perpendicular vibrations (CO_2 and H_2O). fundamental, overtone, combination and difference bands. Fermi resonance. Force constant and its significance. Theory of infrared absorption and theoretical group frequency. Intensity of absorption band and types of absorptions. Correlation chart. Important spectral regions - hydrogen stretching region, double and triple bonds regions, fingerprint region. Factors affecting the group frequency – Physical state, vibrational coupling, electrical effect, hydrogen bonding, steric effect and ring strain. Applications: Structures of small molecules: XY_2 – linear or bent, XY_3 – planar or pyramidal.

[16 HOURS]

UNIT- III

Raman spectroscopy: Introduction, Raman and Rayleigh scattering, Stokes and anti-Stokes lines, polarization of Raman lines, depolarization factor, polarizability ellipsoid. Theories of Raman spectra - classical and quantum theory. Rotation-Raman and vibration-Raman spectra. Comparison of Raman and IR spectra, rule of mutual exclusion principle. Vibration modes of some simple molecules and their activity in Raman.

UV Visible spectroscopy: Quantitative aspects of absorption – Beer's law, Technology associated with absorption measurements. Limitations of the law – real, chemical, instrumental and personal.

NQR Spectroscopy: Quadrupolar nuclei, electric field gradient, nuclear quadrupole coupling constants, energies of quadrupolar transitions, effect of magnetic field. Applications.

Mössbauer spectroscopy: The Mössbauer effect, chemical isomer shifts, quadrupole interactions, measurement techniques and spectrum display, application to the study of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+} compounds, nature of M-L bond, coordination number and structure), detection of oxidation states and inequivalent Mössbauer atoms.

Electron Spin Resonance Spectroscopy: Basic principles, hyperfine couplings, the 'g' values, factors affecting 'g' values, isotropic and anisotropic hyperfine coupling constants, Zero Field splitting and Kramer's degeneracy. Measurement techniques and Applications to simple inorganic and organic free radicals and to inorganic complexes.

[16 HOURS]

References

1. Vibrational Spectroscopy - Theory and Applications- D.N. Sathyanarayana, New Age International Publications, New Delhi (1996).
2. Spectroscopy, B.P. Straughan and S. Walker, John Wiley & Sons Inc., New York, Vol. 1 and 2, 1976.
3. Vibration Spectroscopy Theory and Applications, D.N. Satyanarayana, New Age International, New Delhi.
4. Spectroscopy, B.P. Straughan and S. Salker, John Wiley and Sons Inc., New York, Vol.2, 1976.
5. Organic Spectroscopy, William Kemp, English Language Book society, Macmillan, 1987.
6. Quantum Chemistry – A.K. Chandra. 2nd edition, Tata McGraw Hill Publishing Co. Ltd., (1983).
7. Quantum Chemistry – Eyring, Walter and Kimball. John Wiley and Sons, Inc., New York.
8. Quantum Chemistry – I.N. Levine. Pearson Education, New Delhi, (2000).
9. Theoretical Chemistry – S. Glasstone. East West Press, New Delhi, (1973).
10. Quantum Chemistry – R.K. Prasad, New Age International Publishers, (1996).
11. Valence Theory – Tedder, Murel and Kettle.
12. Quantum Chemistry – D.A. McQuarrie.
13. Theoretical Inorganic Chemistry – Day and Selbin.
14. Fundamentals of Molecular Spectroscopy, C.N. Banwell and E.M. McCash. 4th edition, Tata McGraw Hill, New Delhi.
15. Introduction to Spectroscopy - Pavia, Lampman and Kriz, 3rd edition, Thomson.
16. Spectroscopy, B.P. Straughan and S. Walker, John Wiley & Sons Inc., New York, Vol. 1 and 2, 1976.
17. Vibration Spectroscopy Theory and Applications, D.N. Satyanarayana, New Age International, New Delhi.
18. D. A. McQuarrie and J.D. Simon –Physical Chemistry, VIVA Students Ed. (2003).
19. J. D. Graybeat. Molecular Spectroscopy, McGraw-Hill International Edition (1988). Spectroscopy of Organic Compounds-3rd Ed.-P.S. Kalsi (New Age, New Delhi) 2000.
20. E.A.V. Ebsworth, D.W.H. Ranklin and S. Cradock: Structural Methods in Inorganic Chemistry, Blackwell Scientific, 1991.
21. J. A. Iggo: NMR Spectroscopy in Inorganic Chemistry, Oxford University Press, 1999.
22. C. N. R. Rao and J. R. Ferraro: Spectroscopy in Inorganic Chemistry, Vol I & II (Academic) 1970.
23. Spectroscopy, B. P. Straughan and S. Salker, John Wiley and Sons Inc., New Yourk, Vol.2, 1976.

PRACTICALS – HARD CORE

Analytical Chemistry/ Inorganic Chemistry

[128 HOURS EACH]

Organic Chemistry/ Physical Chemistry

[128 HOURS EACH]

Experiments are as in FIRST SEMESTER. Every student will carry out experiments on a rotation basis in the FIRST and SECOND semesters.

THEORY – SOFT CORE

All the courses are same as that of I Semester and a student can chose any course of his/ her choice provided that the same course has not been studied in the I Semester.

THIRD SEMESTER

THEORY – HARD CORE

CHA HCT: 3.1. INSTRUMENTAL METHODS OF ANALYSIS

UNIT – I

Flame photometry and Atomic absorption spectrometry: Energy level diagrams - atomic absorption spectra. Flame characteristics. Flame atomizers and electrothermal atomization. Comparison of spectral interferences, chemical and physical interferences in FP and AAS. Use of organic solvents. Quantitative techniques - calibration curve procedure and the standard addition technique. Typical commercial instruments for FP and AAS, applications. Qualitative analysis and quantitative evaluations. Relative detectabilities of atomic absorption and flame emission spectrometry.

Molecular luminescence spectrometry: Theoretical basis for fluorescence and phosphorescence. Singlet and triplet excited states. Variables affecting luminescence - quantum efficiency, transition types, structure and structural rigidity, temperature and solvent effects, effect of *pH*, dissolved oxygen and concentration effect. Excitation spectra *vs* emission spectra. Fluorescence instrumentation - fluorimeters and spectrofluorimeters. Sensitivity and selectivity. Modification necessary to measure phosphorescence. General scope of applications of luminescence.

Nephelometry and turbidometry: Principles, instrumentation and applications.

[16 HOURS]

UNIT – II

Classification of electrochemical methods: Controlling and measuring current and potential potentiometers, galvanostats and potentiostats.

Potentiometric methods of analysis. Potentiometric electrochemical cells. The Nernst equation. Liquid junction potentials. Reference electrodes - SHE, calomel electrode and silver/ silver chloride electrode. Metallic indicator electrodes - electrodes of first kind and second kind. Redox electrodes. Membrane electrodes – membrane potential, selectivity of membranes. Glass ion selective electrodes. Crystalline solid state ion selective electrodes. Liquid-based ion selective electrodes. Gas sensing electrodes. Potentiometric biosensors. Quantitative applications. Activity *vs* concentration. Quantitative analysis using external standards and the method of standard additions. Measurement of *pH*. Clinical and environmental applications.

Electrogravimetric analysis: Theory, apparatus, cell processes, deposition and separation, electrolytic separation of metals, applications.

Coulometric methods of analysis: General discussion, coulometry at controlled potential, apparatus and general technique, applications, coulometric titrations (amperometric coulometric) - principles, apparatus, comparison of coulometric titrations with conventional titrations, automatic coulometric titrations, applications.

Voltammetry: Fundamentals of voltammetry. **Cyclic voltammetry:** Principles and applications. **Stripping analysis:** Stripping voltammetry - basic principles, electrodes used for stripping analysis, apparatus for stripping analysis, applications, determination of lead in water voltammetry with micro electrodes.

[16 HOURS]

UNIT – III

Thermal method of analysis: Introduction,

Thermogravimetric analysis (TGA): types of thermogravimetric analysis, principles. Factors affecting the results - heating rate, furnace, instrument control/ data handling. Applications - purity and thermal stability, evaluation of correct drying temperature, analysis of complex mixture and determination of kinetic parameters of thermal degradation.

Differential thermal analysis (DTA): Theory - variables affecting the DTA curves. Differences between TGA and DTA. General principles. Instrumentation. Applications - analysis of the physical mixtures and thermal behaviour study. Determination of melting point, boiling point and decomposition point.

Differential scanning calorimetry (DSC): Basic principle. Differences between DTA and DSC. Instrumentation - power compensated DSC, Heat flux DSC. Applications - studies of thermal transitions and isothermal crystallization. Pharmaceutical industry for testing the purity of the samples.

Thermomechanical analysis. Dynamic mechanical analysis.

Enthalpimetric analysis: Thermometric titrimetry and direct injection enthalpimetry - principle, instrumentation, applications.

[16 HOURS]

References:

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th edition, 2001 John Wiley & Sons, Inc. India.

3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993 Prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003 Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
6. Instrumental Methods of Analysis by H.H. Willard, L.L. Merritt and J.A. Dean, 7th Edition, CBS Publishers, New Delhi, 1988.
7. Principles and Practice of Analytical Chemistry, F.W. Fifield and Kealey, 3rd edition, 2000, Blackwell Sci., Ltd. Malden, USA.
8. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.
9. Introduction to Instrumental Analysis, Braun, Pharm. Med. Press. India.
10. Instant Notes of Analytical Chemistry, Kealey and Haines, Viva Books Pvt. Ltd., New Delhi, 2002.

CHO HCT: 3.2. SPECTROSCOPY

UNIT – I

UV Visible spectroscopy: Introduction, electronic transitions, simple chromophoric groups - systems of extended conjugation - aromatic systems - types of auxochromes - Functions of auxochromes - absorption and intensity shift - types of transitions - transition probability - types of absorption bands - solvent effects and choice of solvent - effect of polarity on various type of bonds Woodward's empirical rules for predicting the wavelength of maximum absorption for conjugated dienes, cyclic trienes and polyenes, α,β -unsaturated aldehydes and ketones, benzene and substituted benzene rings.

IR spectroscopy: Introduction, instrumentation, sample handling, modes of vibrations, Hooke's law, Characteristic group frequencies and skeletal frequencies. Finger print region, Identification of functional groups - alkenes, aromatics, carbonyl compounds (aldehydes and ketones, esters and lactones), halogen compounds, sulphur and phosphorus compounds, amides, lactams, amino acids and amines. Factors affecting group frequencies and band shapes, conjugation, resonance and inductance, hydrogen bonding and ring strain. Tautomerism, *Cis-trans* isomerism. Applications of IR spectroscopy.

[16 HOURS]

UNIT – II

Nuclear magnetic resonance spectroscopy: General introduction and definition, magnetic properties of nuclei (magnetic moment, g factor) and theory of nuclear resonance. Larmor precession frequency, resonance condition and relaxation processes.

Chemical shift: Standards employed in NMR, factors affecting chemical shift, electronegativity, shielding and deshielding mechanism, van der Waals deshielding, H-bonding, diamagnetic and paramagnetic anisotropics. Spin-spin coupling, chemical shift values and correlation for protons bonded to carbon and other nuclei. Instrumentation and sample handling.

Equivalence and magnetic equivalence proton exchange reactions, effects of chiral center, complex spin-spin interaction, stereochemistry, hindered rotation, Karplus curve - variation of coupling constants with dihedral angles. Simplification of complex spectra: isotopic substitution, increasing magnetic field strength, double resonance, spin decoupling, contact shift reagents, FT-NMR: Principle and applications, variable temperature profile, Nuclear Overhauser Effect (NOE).

[16 HOURS]

UNIT – III

¹³C-NMR spectroscopy: Comparison of ¹H-NMR and ¹³C-NMR. Multiplicity - proton decoupling, noise decoupling, off resonance decoupling, selective proton decoupling, noise decoupling by FT mode, chemical shift, application of ¹³C-NMR. ³¹P & ¹⁹F, Two dimensional NMR.

Mass spectroscopy: Principles, instrumentation, different methods of ionization. EI, CI, FD and FAB, Ion separators - single focusing separator with magnetic deflection, double focusing analyzer, time-of-flight separator and quadrupole analyzer, Mass spectra – molecular ion, base peak, meta-stable peak. General rules for fragmentation pattern. Nitrogen rule, ortho effect, Hydrogen transfer rearrangement and McLafferty rearrangement. Mass spectral fragmentation of organic compounds (acids, esters, hydrocarbons, halogenated hydrocarbons, alcohols, carbonyl compounds, amines, ethers and heterocyclic compounds).

Composite problems: Problems involving the application of the above spectroscopic techniques for structural elucidation of organic molecules.

[16 HOURS]

References:

1. Spectroscopy, B.P. Straughan and S. Salker, John Wiley and Sons Inc., New York, Vol.2, 1976.
2. Organic Spectroscopy, William Kemp, English Language Book society, Macmillan, 1987.

3. Application of Absorption Spectroscopy of Organic Compounds, John R. Dyer, Prentice Hall of India Private Ltd., New Delhi, 1974.
4. Spectrometric Identification of Organic Compounds, 4th edition, Robert M. Silverstein, G. Clayton Bassler and Terence C. Morrill, John Wiley & Sons, New York, 1981.
5. Organic Spectroscopy, V.R. Dani, Tata McGraw-Hall Publishing Company Limited, New Delhi. 1995.
6. Interpretation of Carbon-13 NMR Spectra, F.W. Wehrli and T. Wirthin, Heyden, London, 1976.
7. NMR spectroscopy – Powai.
8. Introduction to spectroscopy 3^{ed}, Pavia, Lampman, Kriz.

THEORY – SOFT CORE

CHI SCT 3.1: INORGANIC CHEMISTRY-II

UNIT – I

Ionic solids: Introduction, Characteristic structures of ionic solids (NaCl, CsCl, ZnS, fluorite, rutile, β -cristobalite and cadmium iodide). The rationalization of structures.

The energetics of ionic bonding: Lattice enthalpy and Born-Haber cycle. Calculation of lattice enthalpies. Comparison of experimental and theoretical values of lattice enthalpy. The Kapustinskii equation. Consequences of lattice enthalpies.

Modern concept of acids and bases: Lux-Flood and Usanovich concepts, solvent system and leveling effect. Hard-Soft Acids and Bases, Classification and Theoretical backgrounds.

Supercritical fluids: Properties of supercritical fluids and their uses as solvents. Supercritical fluids as media for inorganic chemistry.

[16 HOURS]

UNIT – II

Biological and Medicinal Applications: Organomercury, boron, silicon and arsenic compounds.

Catalysis: General principles-The language of catalysis. Homogeneous and heterogeneous catalysts.

Homogeneous catalysis: Alkene hydrogenation, hydroformylation, The Wacker's process, Monsanto acetic acid process and L-DOPA synthesis, alkene oligomerizations, water-gas shift reactions. Palladium catalysed C-C bond forming reactions.

Heterogeneous catalysis: Alkene polymerization: Ziegler-Natta catalysis, Fischer-Tropsch carbon chain growth.

Zeolites as catalysts for organic transformation: Uses of ZSM - 5

Alkene metathesis, hydroboration, arylation or vinylation of olefins (Heck reaction).

Hybrid catalysts: Tethered catalysis. Biphasic systems.

Hydrosilylation: Platinum catalyst, Asymmetric palladium catalyst, Rhodium catalysts for asymmetric ketone reduction.

Asymmetric catalysis: General features of chiral ligands and complexes; mechanisms and catalytic cycles in hydrogenation, isomerization, epoxidation and catalytic reactions of C-C bond formation.

[16 HOURS]

References:

1. Basic Organometallic Chemistry - B.D. Gupta and A.J. Elias, Universities Press (2010).
2. Organometallics - A Concise Introduction, 2nd edition, Christoph Elschenbroich and Albert Salzer VCH, (1992).
3. Inorganic Chemistry, 2nd edition, C.E. Housecroft and A.G. Sharpe, Pearson Education Ltd., (2005).
4. Inorganic Chemistry- 3rd edition, G.L. Miessler and D.A. Tarr, Pearson Education, (2004).
5. Inorganic Chemistry, 4th edition. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Oxford University Press (2004).

CHI SCT 3.2: STRUCTURAL METHODS IN INORGANIC CHEMISTRY

UNIT – I

NMR spectroscopy: Basic principles, chemical shift and factors affecting it, coupling constants. ¹⁹F, ³¹P, ¹¹B - NMR and NMR of paramagnetic complexes. Double resonance technique, The Nuclear Overhauser Effect, Magnetic susceptibility measurements by Evan's method. NMR to solids.

ESR spectroscopy: Theory, presentation of the spectrum, hyperfine coupling, the g value and factors affecting the magnitude of the g value. Zero-field splitting and Kramers' degeneracy. Application to simple inorganic and organic free radicals and to metal complexes.

NQR spectroscopy: Theory, energies of the quadrupole transitions, instrumentation, effect of magnetic field on the spectra, relationship between electric field gradient and molecular structures. Applications - interpretation of e^2Qq data, structural information from NQR data.

[16 HOURS]

UNIT – II

Vibrational spectroscopy: Introduction, theory of infrared absorption, theoretical group frequencies, correlation chart. Applications to coordination compounds - aquo, amine, urea, DMSO, *cis* and *trans* metal complexes. Change in spectra accompanying change in symmetry upon coordination (nitrite, sulphate, nitrate, perchlorate and carbonate)

Mossbauer spectroscopy: Theoretical basis, interpretation of Mossbauer spectra - isomer shift, quadrupole splitting and magnetic hyperfine structures. Application: $I_2Br_2Cl_4$, $Fe_3(CO)_{12}$, Prussian blue, nitroprusside, hexacyanoferrate.

Photoelectron spectroscopy: Introduction, principles, chemical shifts, photoelectron spectra of simple molecules, X-ray photoelectron and Auger electron spectroscopy. Applications.

Mass spectrometry: Theory, experimental techniques, molecular ions, fragmentation and ion reaction, Applications to coordination compounds.

[16 HOURS]

References:

1. Electronic Absorption Spectroscopy and Related Techniques – D.N. Sathyanarayana, Universities Press (2001).
2. Structural Methods in Inorganic Chemistry – E.A.V. Ebsworth, D.W.H. Ranklin and Cradock, Blackwell Scientific Publications (1988).
3. Physical Methods in Inorganic Chemistry – R.S. Drago, Saunders Publishers (1966).

CHP SCT 3.2: BIOPHYSICAL CHEMISTRY AND POLYMERS

UNIT – I

Electrokinetic phenomena: Electrophoresis - principles of free electrophoresis, zone electrophoresis, gel electrophoresis and its applications in qualitative and quantitative study of proteins. Determination of isoelectric point of a protein. Electroosmosis and streaming potential and its biological significance. Biological significance of Donnan membrane phenomenon. Micelles and its involvement during digestion and absorption of dietary lipids. Diffusion of solutes across biomembranes and its application in the mechanism of respiratory exchange.

“Salting In” and “Salting Out” of proteins. Osmotic behaviour of cells and osmo-regulation and its application in the evolution of excretory systems of organisms. Effect of temperature and pH on the viscosity of biomolecules (albumin solution). Significance of viscosity in biological systems - mechanism of muscle contraction, detection of intrastrand disulfide bonds in proteins, polymerization of DNA and nature of blood flow through different vessels. Effect of temperature, solute concentration (amino acids) on surface tension. Biological significance of surface tension - stability of Alveoli in lungs, interfacial tension in living cells (Danielli and Davson model). Application of sedimentation velocity and sedimentation equilibrium method for molecular weight determination of proteins.

[16 HOURS]

UNIT – II

Polymers: Fundamentals of polymers - monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers. Polymerization - condensation, addition, free radical, ionic, co-ordination polymerization and ring opening polymerization. Molecular weight and size. Polydispersion. Average molecular weight concepts – number, weight and viscosity average molecular weight. Determination of molecular weights - viscosity method, osmotic pressure method, sedimentation and light scattering method.

Kinetics of Polymerization - condensation, addition, free radical, ionic, co-ordination polymerization. Kinetics of copolymerisation and polymer degradation.

Phase transitions in polymers and thermal characterization: Glass transition, crystallinity and melting- correlation with the polymer structure.

Polymers in solution: Criteria of polymer solubility. Thermodynamics of polymer solutions.

[16 HOURS]

References:

1. Introduction to Physical Organic Chemistry, R.D. Gilliom, Madison – Wesley, USA (1970).
2. Physical Organic Chemistry, Reaction Rate and Equilibrium Mechanism – L.P. Hammett, McGraw HillBook, Co., (1970).
3. Biophysical Chemistry, Principle and Technique – A. Upadhyay, K. Upadhyay and N. Nath, Himalaya Publishing House, Bombay, (1998).
4. Essentials of Physical Chemistry and Pharmacy – H. J. Arnikar, S. S. Kadam, K.N. Gujan, Orient Longman, Bombay, (1992).
5. Text book of polymer Science. F.W. Billmeyer, Jr., John Wiley. London (1994).
6. Polymer Science. V. R. Gowrikar, N. V. Vishwanathan and J. Sreedhar, Wiley Eastern, New Delhi (1990).

7. Fundamentals of Polymer Science and Engineering. A. Kumar and S.K. Gupta, Tata – McGraw Hill New Delhi (1978).
 8. Polymer Characterization, D. Campbell and J. R. White, Chapman and Hall, New York.
 9. Fundamental Principles of Polymer materials, R. L. Rosen, John Wiley, New York.
- Functional monomers and polymers by K. Takemoto, Y. Inaki and P. M. Ottenbrite, Marcel dekker, Inc., New York, 1987.

CHP SCT: 3.4. APPLICATIONS OF CHEMICAL KINETICS AND QUANTUM CHEMISTRY

UNIT - I

Homogenous catalysis: Acid-base catalysis, specific acid and base catalysis. General acid and base catalysis. Oxidation of amino acids and carbohydrates in presence of acid and base catalysis. Acidity functions - Bronstead, Hückel, Hammett and Bunnett hypothesis.

Chain reactions: Rice-Herzfeld mechanism for the thermal decomposition of acetaldehyde, Kinetics of explosive reactions, explosion limits (H_2 and O_2 reaction). Kinetics of autocatalytic and oscillatory chemical reactions, oscillatory chemical reaction of oxidation of malic acid by bromate ion catalyzed by Ce(III). Catalyzed and uncatalyzed reaction: Ru(III) catalyzed oxidation reaction of primary amines by chloramine – T in HCl medium.

[16 HOURS]

UNIT – II

Applications of quantum chemistry: Variation theorem- statement and proof. Application of variation method to He atom, the structure of many electron systems/ atoms (secular equations & determinants), Spin-orbit interaction, antisymmetry and Pauli exclusion principle. Angular momenta (commutations, relations, operators), Term symbols, Russell-Saunders terms and coupling schemes, Slater orbitals and SCF method for many electron systems.

Molecular wave functions: Born-Oppenheimer approximations. Covalent bond –valence bond and molecular orbital approaches with comparisons. MO theory applied to homonuclear and heteronuclear diatomics by LCAO methods, correlation diagrams, non-crossing rule.

Theory of directed valence- hybridization and geometry of molecules in terms of molecular orbitals (bond angle, dihedral angle), localised and delocalised molecular orbitals.

Conjugated and aromatic molecules: Huckel molecular orbital (HMO) theory of linear conjugated systems (ethane & allyl systems) and aromatic molecules (benzene as an example). Calculation of delocalization energies, bond order & charge density.

[16 HOURS]

References:

1. Statistical Thermodynamics by B.C. Mclelland, Chapman and Hall, London (1973).
2. Elementary Statistical Thermodynamics by N.D. Smith, Plenum Press, NY (1982).
3. Elements of Classical and Statistical Thermodynamics by L.K. Nash, Addison-Wesley (1970).
4. Statistical Thermodynamics by I.M. Klotz.
5. Introduction to Statistical Thermodynamics by M. Dole, Prantice Hall, (1962).
6. Text Book of Physical Chemistry by Samuel Glasstone, McMillan Indian Ltd., 2nd edition (1974).
7. Elements of Physical Chemistry by Lewis and Glasstone.
8. Physical Chemistry by P.W. Atkins, ELBS, 4th edition, Oxford University Press (1990).
9. Kinetics and Mechanism of Chemical Transformation by J. Rajaram and J.C. Kuriacose.
10. Chemical Kinetics – L.K. Jain.
11. Chemical Kinetics – Benson.
12. Physical Organic Chemistry, Reaction Rate and Equilibrium Mechanism – L.P. Hammett, McGraw HillBook, Co., (1970).
13. Fundamentals of Photochemistry – Rohatgi and Mukherje (New Age Bangalore) 2000.

PRACTICALS – SOFT CORE

CHA SCP: 3.1. ANALYTICAL CHEMISTRY PRACTICALS

[96 HOURS]

PART – III

1. Determination of calcium in limestone by redox, acid-base and complexation titrations.
2. Determination of vitamin C in orange juice by titration with cerium(IV) and with 2,6-dichlorophenol indophenol.
3. Determination of mercury in an algaecide by EDTA titration; and arsenic in ant control preparation by redox titration.
4. Determination of aluminium and magnesium in antacids by EDTA titration.
5. Analysis of a copper-nickel alloy sample for copper and nickel by EDTA titration using masking and selective demasking reactions.
6. Determination of zinc in a sample of foot powder and thallium in a sample of rodenticide by EDTA titration.
7. Determination of saccharin in tablets by precipitation titration.

- Determination of iodine value and saponification value of edible oils.
- Determination of ascorbic acid in goose berry/bitter gourd by titrimetry and spectrophotometry using *N*-bromosuccinimide (NBS).
- Analysis of a mixture of iron(II) and iron(III) by EDTA titration using *pH* control.
- Determination of sulphadiazole drugs by potentiometry using NaNO_2 and iodometric assay of penicillin.
- Electrolytic determination of copper and lead in brass.
- Polarographic determination of copper and zinc in brass.
- Determination of sodium, potassium and calcium in mineral waters by atomic emission spectrometry.
- Determination of iron in mustard seeds and phosphorus in peas by spectrophotometry.
- Analysis of waste water for anionic detergents and phenol by spectrophotometry.
- Fluorimetric determination of riboflavin (vit. B₂) in tablets.
- Colorimetric analysis of procaine by diazotization and coupling reaction.
- Determination of manganese in steel by extraction-free spectrophotometry and molybdenum in steel by extractive spectrophotometry.

PART – IV

- Analysis of waste waters for DO and COD by titrimetry.
- Analysis of a ground water sample for sulphate by titrimetry (EDTA) and turbidimetry.
- Potentiometric determination of formula and stability constant of a silver-ammonia complex ion.
- Kinetic determination of urinary creatinine and purity of a commercial H_2O_2 sample.
- Determination of chromium(III) and iron(III) in a mixture by kinetic masking methods.
- Catalytic determination of traces of selenium in biological materials and iodide in blood serum.
- Photometric and potentiometric titration of iron(III) with EDTA.
- Photometric and potentiometric titration of copper with EDTA.
- Analysis of brackish water for chloride content by a) spectrophotometry (mercuric thiocyanate method), b) conductometry (silver nitrate) and c) potentiometry (silver nitrate).
- Conductometric titration of sodium acetate with HCl and NH_4Cl with NaOH.
- Ascorbic acid determination in natural orange juice by coulometry.

12. Spectrophotometric determination of iron in natural waters using thiocyanate and 1,10-phenanthroline as reagents.
13. Determination of fluoride in drinking water/ground water by spectrophotometry (alizarin red lake method).
14. Analysis of waste water for
 - a) phosphate by molybdenum blue method
 - b) ammonia-nitrogen by Nessler's method
 - c) nitrite-nitrogen by NEDA method
15. Analysis of a soil sample for
 - a) calcium carbonate and organic carbon by titrimetry.
 - b) calcium and magnesium by EDTA titration.
16. Analysis of a soil sample for
 - a) Available phosphorus by spectrophotometry.
 - b) Nitrate-nitrogen/nitrite nitrogen/ammonia nitrogen by spectrophotometry.
 - c) sodium and potassium by flame photometry.
17. Analysis of urine for
 - a) urea and uric acid by titrimetry and spectrophotometry.
 - b) Sulphate by precipitation titration after ion-exchange separation.
 - c) Sugar by Benedict's reagent.
18. Analysis of blood for
 - a) cholesterol by spectrophotometry
 - b) bicarbonate by acid-base titration.
19. Ultraviolet spectrophotometric determination of aspirin, phenacetin and caffeine in APC tablets using solvent extraction.
20. Fluorimetric determination of quinine in an antimalarial tablet.

References:

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th edition, 2001 John Wiley & Sons, Inc. India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993, prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003 Pearson Education Pvt. Ltd., New Delhi.

5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
6. Pharmaceutical Drug Analysis by Ashutoshkar, New Age International Publishers, New Delhi, 2005.
7. Practical Pharmaceutical Chemistry, Ed. A. H. Geckett, J. B. Stenlake, 4th edition. Part I and II, CBS Publishers, New Delhi.
8. Quantitative Analysis of Drugs in Pharmaceutical Formulations, P. D. Sethi, 3rd edition, CBS Publishers & Distributors, New Delhi, 1997.
9. Practical Clinical biochemistry methods and interpretations, R. Chawla, J.P. Bothers Medical Publishers (P) Ltd., 1995.
10. Laboratory Manual in Biochemistry, J. Jayaraman, New Age International Publishers, New Delhi, 1981.
11. Practical Clinical Biochemistry, Harold Varley and Arnold.Hein mann, 4th edition.
12. Environmental Science: Laboratory Manual, Maurice A. Strabbe, The C.V. Mosbey Co. Saint Loucs, 1972.
13. Experiments on Water Pollution, D.I. Williams and D. Anglesia, Wayland Publishers Ltd., England, 1978.
14. Experiments on Land Pollution, D.I. Williams and D. Anglesia, Wayland Publishers Ltd., England, 1978.
15. Experiments in Environmental Chemistry, P.D. Vowler and D.W. Counel, Pergamon Press, Oxford 1980.
16. Manual Soil Laboratory Testing, vol. I, K.H. Head, Pentech Press, London 1980.

CHI SCP: 3.2. INORGANIC CHEMISTRY PRACTICALS

[128 HOURS]

PART – III

1. Determination of aluminium and bismuth by complexometric titration.
2. Determination of lead and tin in a mixture.
3. Determination of calcium and lead in a mixture by pH control and complexation method.
4. Determination of zinc, manganese and magnesium in a mixture using fluoride as a demasking agent.
5. Quantitative analysis of copper(II) and iron(II) in a mixture:
 - i. Copper gravimetrically as CuSCN and

- ii. Iron volumetrically using cerium(IV) solution
- 6. Determination of iron as the 8-hydroxyquinolate by solvent extraction method.
- 7. Determination of the composition of iron-phenanthroline complex by:
 - (a) Job's method
 - (b) Mole-ratio method and
 - (c) Slope-ratio method.
- 8. Polarographic estimation of cadmium and zinc.
- 9. Spectrophotometric determinations of:
 - a. Titanium using hydrogen peroxide
 - b. Chromium using diphenyl carbazide in industrial effluents
 - c. Nickel using dimethylglyoxime in steel solution
- 10. Solvent extraction of ferric thiocyanate complex and determination by colorimetry.

PART – IV

- 1. Preparation of hexaamminecobalt(III) chloride and estimate cobalt ion.
- 2. Preparation and characterization of:
 - a) Chloropentaammine cobalt(III) chloride
 - b) Estimation of chloride in a complex by potentiometric or ion-exchange method
- 3. Using chloropentaammine cobalt(III) chloride, prepare nitro and nitritopentamine cobalt(III) chloride. Record the IR spectra of the isomers and interpret.
- 4. Preparation of potassium tris-oxalato chromate (III) trihydrate and estimate the metal ion.
- 5. Preparation of mercurytetrathiocyanatocobaltate(II) and estimation of mercury by gravimetry.
- 6. Solid phase synthesis of *trans*-bis glycinato copper(II).
- 7. Synthesis and characterization of *tris*-triphenylphosphine copper (I) nitrate. Estimate copper ion.
- 8. Preparation of bis-dichlorotriphenyl phosphine nickel (II).
- 9. Preparation of hexaamminenickel(II) chloride.
- 10. Demonstration Experiments:
 - (a) Recording and interpretation of IR and NMR spectra of complexes.
 - (b) Spectrochemical series - Evaluation of Dq value.
 - (c) DNA interaction with metal complexes by UV-visible absorption and viscosity methods.

References:

1. Advanced Physico-Chemical Experiments – J. Rose.
2. Instrumental Analysis Manual - Modern Experiments for Laboratory – G.G. Guilbault and L.G. Hargis.
3. A Text Book of Quantitative Inorganic Analysis – A.I. Vogel, 5th edition.
4. Experimental Inorganic Chemistry – G. Palmer.
5. Inorganic Synthesis – O. Glemser.
6. Experimental Inorganic/ Physical Chemistry- Mounir A. Malati.
7. Quantitative Chemical Analysis – Daniel C. Harris, (2006) 7th edition.
8. Spectrophotometric Determination of Elements – Z. Marczenko

CHO SCP: 3.3. ORGANIC CHEMISTRY PRACTICALS

[128 HOURS]

PART – III

Multi step synthesis

1. Oxidation of cyclohexanol to adipic acid via cyclohexanone
2. Esterification: Preparation of benzocaine from *p*-nitrotoluene
3. Diazotization (Sandmeyer's reaction): Preparation of *p*-chlorobenzoic acid from *p*-toluidine
4. Molecular rearrangement:
 - i. Preparation of *o*-chlorobenzoic acid from phthalic anhydride
 - ii. Preparation benzilic acid from benzaldehyde
 - iii. Preparation of *o*-hydroxy benzophenone from phenyl benzoate via Fries rearrangement
 - iv. Preparation of benzanilide from benzophenone oxime via Beckmann rearrangement.
5. Grignard reaction: Preparation of triphenyl carbinol
6. Preparation of luminol from phthalic anhydride
7. Synthesis of isoxazolines and pyrazolines via 1,3-dipolar cycloaddition.
8. Solvothermal synthesis
9. Synthesis of tetralones starting from aryl aldehydes.
10. Synthesis of *m*-chloriodobenzene from *m*-dinitrobenzene
11. Synthesis of Schiff base from nitro compound.

PART – IV

Isolation of natural products

1. Fractional crystallization: separation of mixture of naphthalene and biphenyl
2. Fractional distillation: Separation of mixture of hexane and toluene.
3. Thin layer chromatography: Separation of plant pigments
4. Column chromatography: Separation of mixture of *o* and *p*-nitro anilines
5. Isolation of piperine from pepper
6. Isolation of caffeine from tea
7. Isolation of azeleic acid from castor oil
8. Isolation of clove oil from clove
9. Estimation of sugars by Fehlings method
10. Determination of enol content by Meyer's method
11. Estimation of ketones by haloform reaction
12. Estimation of sugars by Bertrand's method
13. Estimation of nitro groups
14. Estimation of protein by biuret method

Spectral analysis: Structural elucidation of some simple organic compounds by UV, IR, NMR and mass. The spectra have to be provided by the teachers.

References:

1. Manual of Organic Chemistry - Dey and Seetharaman.
2. Modern Experimental Organic Chemistry by John H. Miller and E.F. Neugil, p 289.
3. An Introduction to Practical Organic Chemistry - Robert, Wingrove etc.
4. A Text Book of Practical Organic Chemistry – A.I. Vogel, Vol.III
5. Practical Organic Chemistry - Mann & Saunders
6. Semimicro Qualitative Organic Analysis by Cheronis, Entrikin and Hodnet .
7. R.K. Bansal, Laboratory Manual of Organic Chemistry, New Age International (P) Ltd. London, 3rd edition, 1996.

CHP SCP: 3.4. PHYSICAL CHEMISTRY PRACTICALS

[128 HOURS]

PART – III (NON-INSTRUMENTAL)

1. Determination of energy of activation and thermodynamic activation parameters (ΔH^\ddagger , ΔS^\ddagger , ΔG^\ddagger) for reaction between sodium formate and iodine.
2. To study the kinetics of reaction between acetone and iodine - determination of order of reaction w.r.t. iodine and acetone.
3. Kinetics of decomposition of benzene diazonium chloride, determination of energy of activation and thermodynamic parameters.
4. Kinetics of decomposition of diacetone alcohol by NaOH - determination of energy of activation.
5. To determine the eutectic point of a two component system (Naphthalene-*m*-dinitrobenzene system).
6. Study of phase diagram of a three component system (e.g. acetic acid-chloroform water and system). Construction of binodal curve and indicating tie line.
7. Determination of heat of solution and lattice energy of calcium chloride.
8. To study oscillating or periodic or rhythmic reactions of malonic acid.
9. Determination of partition co-efficient of acetic acid in water and butanol.
10. Determination of activation energy of potassium persulfate and KI.

PART IV (INSTRUMENTAL)

1. Kinetics of saponification of ethyl acetate by conductivity method and study the effect of dielectric constant of the medium (using CH₃OH).
2. Spectrophotometric analysis of a mixture of (a) KMnO₄ and K₂Cr₂O₇.
3. Determination of ionic product of water and study the effect of temperature.
4. Coulometric titration I₂ vs Na₂S₂O₃.
5. Conductometric study of charge transfer complex of p-phenylene diamene with phthalic acid.
6. Determination of mean ionic activity coefficient of a weak electrolyte (acetic acid) by conductometric measurements.
7. Determination of pK value of an indicator (methyl orange).
8. Potentiometric titration of mixture of KCl+KBr+KI vs AgNO₃.

9. Photolysis of CAT.

10. Preparation and UV-visible studies on solid-state materials: a) NiO b) $ZnFe_2O_4$ or $NiFe_2O_4$

c) Fe_3O_4 d) $BaZrO_3$.

References:

1. Practical Physical Chemistry – A.J. Findlay.
2. Experimental Physical Chemistry – F. Daniels *et al.*
3. Selected Experiments in Physical Chemistry – Latham.
4. Experiments in Physical Chemistry – James and Prichard.
5. Experiments in Physical Chemistry – Shoemaker.
6. Advanced Physico-Chemical Experiments – J. Rose.
7. Practical Physical Chemistry – S.R. Palit.
8. Experiments in Physical Chemistry – Yadav, Geol Publishing House.
9. Experiments in Physical Chemistry – Palmer.
10. Experiments in Chemistry – D.V. Jahagirdar, Himalaya Publishing House, Bombay, (1994).
11. Experimental Physical Chemistry – Das. R.C. and Behera B, Tata Mc Graw Hill.

THEORY – OPEN ELECTIVE

CH OET : SELECTED TOPICS IN CHEMISTRY

UNIT – I

Solvent extraction: Basics of solvent extraction principal and application of solvent extraction.

Purification techniques: Crystallization, fractional crystallization, distillation techniques (simple distillation, steam distillation, distillation under reduced pressure, fractional distillation).

Chromatography: Definition, terms, classification of chromatographic techniques, principles of column and planar chromatography

Column chromatography: gas chromatography, high performance liquid chromatography, ion exchange chromatographic method.

Planar chromatography: Paper chromatography and TLC principles, mechanism of separation and application.

Electrophoretic methods: principles, definition, terms, types and applications.

[16 HOURS]

UNIT – II

An overview of metals in Biology: Introduction, the element content of living systems, biological chemistry of hydrogen, the economical use of resources- abundance and availability. Biological need for and the behaviors of inorganic elements.

Basic coordination chemistry for biologists: Introduction, ionic bonding, covalent bonding, coordination geometry, crystal field and ligand field theory.

Metal assimilation pathways: Introduction, metal assimilation in bacteria, plants, fungi and in mammals (iron, copper and zinc).

Metals in medicine: Introduction, *cis*-platin, radioactive pharmaceuticals, lithium compounds in therapy.

[16 HOURS]

UNIT – III

Chemistry of natural products: Carbohydrates (classification and structure of glucose, fructose, galactose, sucrose, maltose and lactose, carbohydrates as source of energy and breakdown process.

Proteins: amino acids classification and structure of α -amino acid, zwitter ion, isoelectric point and its determination by electrophoretic method, Elementary aspect of primary and secondary structures.

Vitamins: Classification, importance of vitamin A, D, E, K, B & C.

[16 HOURS]

UNIT – IV

Thermodynamics: First and second laws of thermodynamics. Concept of entropy and free energy, entropy as a measure of unavailable energy. Entropy and free energy changes and spontaneity of process. Variation of free energy with temperature and pressure. **Chemical kinetics:** Factor affecting the rate of reaction. Order of reaction and its determination. Energy of activation and its determination. Assumption of activated complex theory. **Electrochemistry:** Arrhenius theory of strong and weak electrolytes. Assumptions of Debye-Huckel theory of strong electrolytes. Electrode potential and construction of electrochemical cells. Corrosion and its prevention. **Photochemistry:** Laws of photochemistry, quantum yield and its determination, photodegradation.

[16 HOURS]

References:

1. Arthur I Vogel, Elementary Practical Organic Chemistry, Part I, II and III, CBS Publishers and Distributors, New Delhi, India.
2. I.L. Finar, Organic Chemistry, ELBS Longmann, Vol. I and II, 1984.
3. S K. Ghosh, Advanced General Organic Chemistry, Book and Allied (P) Ltd, 1998.
4. Organic Spectroscopy, William Kemp, English Language Book society, Macmillan, 1987.
5. Application of Absorption Spectroscopy of Organic Compounds, John R. Dyer, Prentice Hall of India Private Ltd., New Delhi, 1974.
6. Spectrometric Identification of Organic Compounds, 4th edition, Robert M. Silverstein, G. Clayton Bassler and Terence C. Morrill, John Wiley & Sons, New York, 1981.
7. Basic Inorganic Chemistry- 3rd edition, F.A. Cotton, G. Wilkinson and P.L. Gaus, John Wiley and Sons, (2002).
8. Inorganic Chemistry Principles of Structure and Reactivity: James E. Huheey, Ellen A. Keiter, Richard L. Keiter, Okhil K. Medhi, Delhi University, New Delhi (2006)
9. Elements of Physical Chemistry – Lewis and Glasstone.
10. Physical Chemistry by P.W. Atkins, ELBS, 4th edition, Oxford University Press (1990).
11. Basic Physical Chemistry by W.J. Moore, Prentice Hall, New Delhi, (1986).
12. Physical Chemistry – G.M. Barrow, McGraw Hill International Service (1988).

FOURTH SEMESTER

THEORY – HARD CORE

CHI HCT: 4.1. BIOINORGANIC CHEMISTRY

UNIT – I

Structural and molecular biology: Introduction, The structural building blocks of proteins, the structural building block of nucleic acids. Metal ion interactions with nucleosides and nucleotides.

General features of DNA - metal complex interaction.

Bioenergetics: Introduction, Redox reactions in metabolism, the central role of ATP in metabolism. Kinetic stability of ATP, Mitochondrial flow of electrons from NADH to O₂. Oxidative phosphorylation and respiratory chain.

Sodium and potassium-channels and pumps: Introduction, transport across membranes. Potassium and sodium channels, The sodium-potassium ATPase, Macro cyclic crown ether compounds, cryptands and ionophores.

Biochemistry of calcium: Introduction - comparison of Ca²⁺ and Mg²⁺. Biological roles of calcium, binding sites of calcium and proteins, storage of calcium, calcium in muscle contraction, calcium in blood clotting process.

Vitamin B₁₂ and Coenzymes: Structural feature, names of different forms, chemistry of cobalamin, biochemical functions of cobalamins, model compounds. Special characteristics of B₁₂ co-enzyme.

[16 HOURS]

UNIT – II

Metal ion transport and storage:

Iron storage and transport: Transferrin, ferritin, phosvitin and gastroferrin.

Iron transport in microbes: siderophores, *in vivo* microbial transport of iron

Oxygen transport and oxygen uptake proteins: Properties of dioxygen (O₂): Thermodynamic and kinetic aspects of dioxygen as an oxidant, activation of dioxygen through complexation with metal ions.

Haemoglobin (Hb) and Myoglobin (Mb) in oxygen transport mechanism: Introduction to porphyrin system, substituent effects on porphyrin rings, functions of Hb and Mb. Characteristics

of O_2^- binding interaction with Hb and Mb. Model compounds for oxygen carriers (Vaska's complex and cobalt(III) – Schiff base complexes). Hemerythrin and hemocyanin.

Electron transport proteins and redox enzymes: Iron – sulfur proteins (rubredoxins and ferredoxins) and cytochromes including cytochrome P450. Catalase and peroxidase: Structure and reactivity.

Superoxide dismutase: Structure and reactivity.

Molybdenum containing enzymes: Aspects of molybdenum chemistry, Xanthine oxidase, aldehyde oxidase, sulfite oxidase, nitrogenase and nitrite reductase.

Non-redox metalloenzymes - Structure and reactivity: Carboxypeptidase-A, alcohol dehydrogenase, leucine aminopeptidase and carbonic anhydrase.

[16 HOURS]

UNIT - III

Therapeutic uses of Metals - Metals in medicine: Introduction, metals and human biochemistry, general requirements.

Disease due to metal deficiency and treatment: Iron, zinc, copper, sodium, potassium, magnesium, calcium and selenium.

Metal complexes as drugs and therapeutic agents: Introduction, antibacterial agents, antiviral agents, metal complexes in cancer therapy, metal complexes for the treatment of rheumatoid arthritis, vanadium diabetes, metal complexes as radio diagnostic agents.

Treatment of toxicity due to inorganics: General aspects of mechanism of metal ion toxicity, (i) Mechanism of antidote complex with poison, rendering it inert: arsenic, lead, mercury, iron, copper.

(ii) Antidote accelerated metabolic conversion of poison to non-toxic product: cyanide and carbon monoxide.

[16 HOURS]

References:

1. The Inorganic Chemistry of Biological Process- 2nd edition, M. N. Hughes, John Wiley and Sons, (1988).
2. Bioinorganic Chemistry - R.W. Hay, Ellis Horwood Ltd., (1984).
3. Biological Inorganic Chemistry – An Introduction, R.R. Crichton, Elsevier, (2008).
4. Bioinorganic Chemistry - A.K. Das, Books and Allied (P) Ltd, (2007).
5. Bioinorganic Chemistry - K. Hussain Reddy, New Age International Ltd. (2003).
6. Bioinorganic Chemistry: A Survey - Eiichiro Ochiai, Academic Press, (2008).

7. Bioinorganic Chemistry: A Short Course - 2nd edition, R.M. Roat-Malone, Wiley Interscience, (2007).
8. Medicinal Applications of Coordination Chemistry - Chris Jones and John Thornback, RSC Publishing, (2007).
9. Transition Metal Complexes as Drugs and Chemotherapeutic Agents - N. Farrell, Kluwer Academic Publishers (1989).
10. The Biological Chemistry of the Elements: The Inorganic Chemistry of Life - 2nd edition, J.J.R. Frausto da Silva and R.J.P. Williams, Oxford University Press, (2001).

CHP HCT: 4.2 ADVANCED PHYSICAL CHEMISTRY

UNIT – I

Kinetics and Thermodynamics of Polymerization: Kinetics of addition, condensation and radiation induced polymerization. Thermodynamics of polymer solutions, The Flory-Huggins Theory, Flory Krigbaum and modified Flory-Huggins Theory.

Copolymerization: Kinetics of copolymerization, Copolymer equation, Monomer reactive ratios. Properties of Polymers: Crystalline melting point and the glass transition temperature.

Polymer molecular weights: Molecular weight distribution, Number average and Weight average molecular weight. Methods for determination of molecular weight – Osmometry-membrane osmometry, vapour pressure osmometry, light scattering, viscosity, ultracentrifugation.

Conducting Polymers: Structure, properties, characterization and applications.

Polymer Degradation, Stability and Environmental Issues: Types of degradation, Thermal degradation, Mechanical degradation, Photodegradation, Degradation by high energy radiation. Chemical, hydrolytic and UV stability. Recycling and biodegradation.

Solid State Chemistry:

Fundamentals of X- Ray Crystallography, law of interfacing angles, law of symmetry, miller indices, Bragg equation (derivation), Experimental methods-powder and rotating crystal photographs.

[16HOURS]

UNIT – II

Photochemistry: Introduction to photochemistry, quantum yield and its determination, factors affecting quantum yield, Actinometry - Uranyl oxalate and potassium ferrioxalate actinometers, acetone and diethylketone actinometers. Term symbols and significance. Photosensitization: by mercury, dissociation of H_2 . Photochemical kinetics of: Decomposition of CH_3CHO , formation of HCl . Photodegradation: Photocatalyst – ZnO , TiO_2 , principle, application of ZnO/ TiO_2 in the photo degradation of dyes (IC), pesticides (DDT) and in industrial effluents. Effect of photo degradation on COD value.

Mechanism of absorption and emission of radiation: Einstein's treatment, selection rules, Life times of excited electronic states of atoms and molecules Types of electronic transitions in organic molecules photochemical pathways, Jablonski diagram, Fluorescence, Phosphorescence. Fluorescence emission, factors affecting fluorescence, viz. structure, solvent, pH, temperature etc. Triplet state and phosphorescence.

Photophysical kinetics: kinetics of unimolecular processes, delayed fluorescence mechanisms, kinetics of collisional quenching, Stern-Volmer equation, quenching by added substances charge transfer mechanism, energy transfer mechanism.

[16 HOURS]

UNIT – III

Irreversible electrode process: Introduction, reversible and irreversible electrodes, reversible and irreversible cells. Polarization, over voltage - ohmic over voltage, concentration over voltage activation over voltage, experimental determination of over voltage. Equations for concentration over potential, diffusion current – stationary current, potential curves, thickness of diffusion layer, diffusion controlled current – potential curves at a dropping mercury electrode, polarography, half wave potential, application in qualitative and quantitative analysis. Energy barrier and electrode kinetics, Butler-Volmer equation, Tafel equation. Hydrogen over voltage and Oxygen over voltage. Effect of temperature, current density and pH on over voltage.

Corrosion: Manifestations of corrosion, types of corrosion, basis of electrochemical corrosion, theories of corrosion. Local cell theory (Wagner and Traud theory), Current – potential relations (Evan diagram) in corrosion cells. Effect of pH, nature of metal and dissolved oxygen (principle of differential aeration) on corrosion. Corrosion inhibition and prevention by painting,

phosphating and by using biomaterials, corrosion protection by anodic (passivation) and cathodic protection.

[16 HOURS]

References:

1. Polymer Science and Technology by Joel R. Fried Third edition, 2002.
2. Polymer Science, V.R.Gowarikar , N.V.Vishwanathan and Jaydev Sreedhar Reprint edition, 2002.
3. Text book of Polymer Science, Fred W. Billmeyer Jr. Third edition, 2000.
4. Principles of Polymerization, George Odian, Third edition 2002.
5. Handbook on Conducting Polymers – T.A.Skotheim, Ed Marcel Dekker Inc, New York, 1 and 2, 1986.
6. Introduction to Solids – Azaroff.
7. Solid State Chemistry and its applications – A.R. West.
8. Principles of the Solid State – H.V. Keer.
9. Basic Solid State Chemistry, 2nd edition, Anthony R. West.
10. Solid State Chemistry: An Introduction, 3rd edition, Lesley E. Smart and Elaine A. Moore.
11. Introduction to Solid state Physics—C. Kittel, 5th edition, Wiley Eastern, Limited.
12. C.N.R. Rao and J. Gopalakrishna “New Directions in solid state chemistry” Cambridge University Press, Cambridge (1999).
13. Essentials of Nuclear Chemistry, H. J Arnika, Wiley Eastern Limited, 4th Edition, (1995).
14. Nuclear and Radiochemistry, G. Friedlander, J. W. Kennedy and J. M. Miller, John Wiley (1981).
15. Introduction to Radiation Chemistry, J. W. T. Spinks and R. J. Woods, John Wiley (1990)
16. Introduction to Nuclear Physics and Chemistry, B.G. Harvey, Prentice hall (1963).
17. Sourcebook on Atomic Energy-S. Glasstone, Van Nostrand Company (1967).
18. Radiochemistry and Nuclear methods of analysis-W.D.Ehman and D.E. Vance, John Wiley (1991).
19. Fundamentals of photochemistry by K.K.Rohatgi-Mukherjee, New Age International Publishers Revised Edition (Reprint 2003).
20. Chemistry and light by Paul Suppan, The Royal Society of Chemistry.

21. Quantum Chemistry – D.A. McQuarrie.
22. Principles and Applications of Electrochemistry–Crow (Chapman hall, London) 1988.
23. Introduction to Electrochemistry by S. Glasstone.
24. Physical Organic Chemistry, Reaction Rate and Equilibrium Mechanism – L. P. Hammett, McGraw HillBook, Co., (1970).
25. Biophysical Chemistry, Principle and Technique – A. Upadhyay, K. Upadhyay and N. Nath, Himalaya Publishing House, Bombay, (1998).
26. Introductory Quantum Chemistry – A.K.Chandra (Tata McGraw Hill) 1994.
27. Introduction to Physical Organic Chemistry, R. D. Gilliom, Madison – Wesley, USA (1970).
28. Quantum Chemistry – Eyring, Walter and Kimball. John Wiley and Sons, Inc., New York.
29. Quantum Chemistry –I.N. Levine. Pearson Education, New Delhi, (2000).
30. Theoretical Chemistry – S. Glasstone. East West Press, New Delhi, (1973).
31. Quantum Chemistry – R.K. Prasad, New Age International Publishers, (1996).
32. Valence Theory – Tedder, Murel and Kettle.

THEORY – SOFT CORE

CHA SCT: 4.1 APPLIED ANALYSIS II

UNIT – I

Soil Analysis: Inorganic and organic components of soil, collection and preparation of soil samples for analysis. Measurement of soil pH and conductivity. Determination of organic carbon, total nitrogen, 53 available nitrogen, ammonia nitrogen, nitrate nitrogen and nitrite nitrogen. Available phosphorus and sulphur-their determination. Analysis of soil for sodium, potassium and calcium and magnesium. Micronutrient elements and their analysis. Pesticide residues in soil, their separation and determination.

Fuel analysis- Fuels and their classification. Solid fuels and their classes - natural, artificial and industrial solid fuels. Coal and its analysis - proximate analysis and ultimate analysis. Liquid fuels and their types. Aniline point, flash point and fire point and their determination, octane number of liquid fuels. Gaseous fuels and their classes, advantages. Combustion of a

carbonaceous fuel – flue gas. Analysis of flue gas or automobile exhaust for CO₂, CO, O₂ and N₂ by Orsat's apparatus. Calorific value of fuel - net and gross calorific values. Determination of calorific value of solid and liquid fuels by bomb calorimeter method.

[16 HOURS]

UNIT - II

Biomedical and forensic analysis: Composition of body fluids and detection of abnormal levels of certain constituents leading to diagnosis of disease. Sample collection and preservation of physiological fluids. Analytical methods for the constituents of physiological fluids (blood, serum, urine).

Blood - estimation of glucose, cholesterol, urea, haemoglobin and bilirubin.

Urine - urea, uric acid, creatinine, calcium phosphate, sodium, potassium and chloride.

Biological significance, analysis and assay of enzymes (pepsin, monoaminoxidase, tyrosinase); and hormones (progesterone, oxytocin, insulin). Chemical, instrumental and biological assays to be discussed wherever necessary.

Forensic analysis: General discussion of poisons with special reference to mode of action of cyanide, organophosphates and snake venom. Estimation of poisonous materials such as lead, mercury and arsenic in biological materials.

[16 HOURS]

CHA SCT: 4.2 APPLIED ANALYSIS III

UNIT – I

Kinetic methods of analysis: Introduction, basis of kinetic methods, rate law expressions. Classifying chemical kinetic methods – direct-computation integral methods, direct-computation rate methods, curve-fitting methods. Instrumentation. Quantitative applications - enzyme catalyzed reactions, non-enzyme catalyzed reactions, non-catalytic reactions. Determining V_{max}, K_m for enzyme catalyzed reactions. Elucidating mechanism for the inhibition of enzyme catalysis. Determination of enzymes, LDH, GOT and GPT. Determination of substrates – urea, uric acid, blood glucose and blood alcohol. Analysis of closely related compounds - neglect of reaction of slow reacting component method and logarithmic extrapolation method.

Automated methods of analysis: An overview. Principles of automation. Automated instruments: process control. Continuous analyzers. Discrete autoanalyzers. Instruments used in automated process control. Automatic instruments - discrete and continuous flow sampling instruments. Flow injection analysis – principles - dispersion co-efficient. Factors affecting peak height, sample volume, channel length and flow rate, and channel geometry. Applications -

limited dispersion applications, medium dispersion applications, stopped flow methods and flow injection titrations. Discrete automatic systems - centrifugal fast scan analyzer, automatic organic elemental analyzers.

Analysis based on multilayer films-general principles, film structures, instrumentation, performance and applications – blood urea nitrogen, blood glucose and potassium.

[16 HOURS]

UNIT – II

Radiometric methods: Radioactive isotopes. Nuclear emissions - α and β -particles, neutrons, gamma rays and miscellaneous nuclear particles. Nuclear reactions, radiochemical decay and activity. Instrumentation and measurement of radioactivity. Radiation detectors - gas ionization, scintillation and semiconductor detectors. Pulse height analysis. Autoradiography. Statistics of radioactive measurements.

Radiochemical analysis: Neutron activation methods - neutrons and their sources. Interaction of neutrons with matter. Theory, experimental considerations and applications. **Isotope dilution methods** - direct isotope dilution and inverse isotope dilution methods and their applications. Radiometric titrations. Radiorelease methods. Radioactive tracers.

Radio immunoassay: Principles of immunoassay. Specificity of immuno assays. Preparation of the antibody, incubation period for the assay, separation of the bound and free antigen. Fluorescence immunoassay. Enzyme immunoassay.

[16 HOURS]

References:

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th edition, 2001 John Wiley & Sons, Inc. India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993 Prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003 Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
6. Instrumental Methods of Analysis by H.H. Willard, L.L. Merritt and J.A. Dean, 7th edition, (1988).
7. Principles and Practice of Analytical Chemistry, F.W. Fifield and Kealey, 3rd edition, 2000, Blackwell Sci., Ltd. Malden, USA.

8. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.
9. Introduction to Instrumental Analysis, Braun, Pharm. Med. Press. India.
10. Instrumental Method of Analysis, W. M. Dean and Settle, 7th edition, 1986, CBS Publishers, New Delhi.
11. Instant Notes of Analytical Chemistry, Kealey and Haines, Viva books Pvt. Ltd., 2002.
12. Soil Chemical Analysis, M.L. Jackson, Prentice Hall of India Pvt. Ltd., New Delhi, 1973.
13. Clinical Chemistry, Principles and Procedures, J.S. Annino, 2nd edition, Boston: Little, Brown, 1960.
14. Methods of Geochemical Analysis, D. Click, Ed., A Multi volume series, New York, Interscience.
15. Clinical Chemistry, Principles and Techniques, R.J. Henry, D.C. Cannon and J.W. Winkleman, Eds., 2nd edition, Hagerstorm, M.D: Harper and Row, 1974.
16. Fundamentals of Clinical Chemistry, N.W. Tietz, Ed., 2nd edition, Philadelphia: W.B. Saunders, 1976.

CHO SCT: 4.3. RETROSYNTHESIS AND ORGANOMETALLIC CHEMISTRY

UNIT – I

Protecting groups: Protection of hydroxyl, carboxyl, carbonyl, thiol and amino groups. Illustration of protection and deprotection in synthesis.

Named reactions: Keto-enol tautomerism, mechanism and synthetic applications of aldol condensations, Claisen reaction, Schmidt reaction, Perkin reaction, Knoevenagel, benzoin and Stobbe condensation, Darzens glycidic ester condensation, Cannizaros reaction, Tischenko reaction. Michael addition, Robinson's annulation reaction.

Retrosynthesis: Introduction to disconnection approach: Basic principles and terminologies used in disconnection approach. One group C-X and two group C-X disconnections. Synthons and synthetic equivalents.

Retrosynthesis and synthesis of benzofurans, *p*-methoxy acetophenone, saccharine, α -bisabolene, nuciferal, penicillin-V.

[16 HOURS]

UNIT - II

Chemistry of organometallic compounds: Synthesis and reactions of organolithium (n-BuLi, PhLi) and organomagnesium (Grignard reagent) compounds.

Organoaluminium reagents: Preparation, site selective and stereoselective additions of nucleophiles mediated by organoaluminum reagents, reaction with acid chlorides, allyl vinyl ethers, 1,2-addition to imines and application in the synthesis of natural products.

Organopalladium compounds: Suzuki coupling, Heck reaction.

Organotin reagents: Barton decarboxylation reaction, Barton deoxygenation reaction, Stille coupling, Stille-Kelley coupling reactions, Barton McCombie reaction, Keck stereoselective allylation and other applications.

Organozinc reagents: Preparation - oxidative addition and transmetallation, addition reactions of alkyl, aryl, allylic and propargylic zinc reagents, diastereoselective and enantioselective addition reaction with aldehydes, Reformatsky reaction.

[16 HOURS]

References:

1. H. Pine, Hendrickson, Cram and Hammond, Organic Chemistry, Mac Grow Hill, New York, 1987.
2. Organic Chemistry - Morrison and Boyd
3. Organic Chemistry- Crabtree
4. Organic Chemistry- Clayden
5. I.L. Finar, Organic Chemistry, ELBS Longmann, Vol. 1 & II, 1984.
6. J. March, Advanced Organic Chemistry, Wiley Interscience, 1994.
7. E.S. Gould, Mechanism and Structure in Organic Chemistry, Halt, Rinhart & Winston, New York, 1964.
8. F.A. Carey and Sundberg. Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York. 1990.
9. Principles of Organic Synthesis - ROC Norman and Coxon.
10. S.K. Ghosh, Advanced General Organic Chemistry, Book and Allied (P) Ltd. 1998.

CHO SCT: 4.4. BIOMOLECULES AND NATURAL PRODUCTS

UNIT - I

Amino Acids: General structure, Physiological properties

Peptides: Structure and conformation of peptide bond, peptide synthesis: Solution phase and Merrifield's solid phase synthesis, Racemization and use of HOBt, Synthesis of oxytocin and vasopressin, biological importance of insulin, selective cleavage of polypeptide bonds (chemical and enzymatic).

Proteins: Structure determination: C and N terminal residue determination, primary, secondary, tertiary and quaternary structure determination, denaturing and renaturing of proteins.

Nucleic acids: Introduction, structure and synthesis of nucleosides and nucleotides, Solid phase synthesis of oligonucleotides, Structure of RNA and DNA, Crick-Watson model, role of nucleic acids in the biosynthesis of proteins.

[16 HOURS]

UNIT – II

Carbohydrates: Synthesis, industrial and biological importance of glycosides, amino sugars, sucrose, maltose and lactose.

Polysaccharides: General methods of structure elucidation. Industrial importance and biological importance of cellulose, starch, glycogen, dextran, hemicellulose, pectin, agar-agar. Photosynthesis and biosynthesis of carbohydrates.

Lipids: Nomenclature, classification, purification, synthesis of lipids, phospholipids, sphingolipids, biological importance of lipids: Lecithin, sphingolipids, oils and fats.

Terpenoids: Introduction, classification (natural and essential oils), isoprene rule and biological importance of terpenoids.

[16 HOURS]

References:

1. I. L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
2. Essentials of physiological chemistry – Anderson, John Wiley & Sons, New York, 1953.
3. K. Albert, L. Lehninger, D.L. Nelson, M.M. Cox, Principles of Biochemistry, CBZ publishers, 1st edition, New Delhi, 1993.
4. Harper's Biochemistry, Ed. R. Harper, 22nd edition, Prentice Hall Press, New York, 1990
5. Carbohydrates – Chemistry and Biochemistry by Pigmann and Harton.
6. An introduction to carbohydrate chemistry by Guthrie and Honeyman.
7. Protein chemistry by Neurath, Vol. I, II and III.
8. Peptide chemistry by Bodanski, Vol. I, II and III.
9. Introduction to the chemistry of fats and fatty acids by F. D. Gunstone.

PRACTICALS – SOFT CORE

Analytical Chemistry/ Inorganic Chemistry

[128 HOURS EACH]

Organic Chemistry/ Physical Chemistry

[128 HOURS EACH]

Experiments are as in THIRD SEMESTER. Every student will carry out experiments on a rotation basis in the THIRD and FOURTH semesters.