CHOICE BASED CREDIT SYSTEM
CONTINUOUS ASSESSMENT GRADING PATTERN (CBCS-CAGP)

VERSION - IV

UNIVERSITY OF MYSORE

Department of Studies in Chemistry

Manasagangotri Mysuru –570 006

REVISED SYLLABUS FOR M. Sc. DEGREE PROGRAMME

2019-20

GUIDELINES AND REGULATIONS LEADING TO MASTER OF SCIENCE IN CHEMISTRY (TWO YEARS - SEMESTER SCHEME UNDER CBCS-CAGP)

Programme details

Name of the Department	:	Department of Studies in Chemistry
Subject	:	Chemistry
Faculty	:	Science and Technology
Name of the Programme	:	Master of Science (M. Sc.)
Duration of the Programme	:	2 years- divided into 4 semesters

Programme objectives

- To provide the latest subject matter both theory as well as practicals in such a way to foster their core competency and discovery learning. A chemistry post graduate as envisioned in this framework would be sufficiently competent in the field to understand further discipline specific studies as well as to begin domine related employment.
- To mould a responsible citizen who is aware of most basic domain-independent knowledge including critical thinking and communication.
- Enable the graduate to prepare for national as well as international competitive examinations, especially UGC-CSIR NET and UPSC civil service examinations.

Programme outcome

- Students will have a strong foundation in the fundamentals and applications of current theoretical and practical chemistry including those in Analytical, Inorganic, Organic and Physical Chemistry.
- Students will be able to design and carry out scientific experiments and accurately record and analyze the results of the experiments.
- Students will be skilled in problem solving, critical thinking and analytical reasoning as applied to scientific problems.
- Students will be able to explore new areas of research in both chemistry and allied fields such as Biochemistry, Material Chemistry, Pharmaceutical chemistry and chemical biology and related technology.
- Students will understand the central role of chemistry to our society which includes understanding of safe handling of chemicals, environmental issues and key issues facing our society in energy, health and medicine.

Programme Specific outcome

- Global level research opportunities to pursue Ph. D. programme, targeted approach of CSIR – NET and competitive civil service examinations.
- Enormous job opportunities at all levels of teaching, chemical, pharmaceutical, food products, life oriented material industries.
- Specific placements in R & D and many pharmaceutical & other industries.
- Facile development for the synthesis of biologically significant organic molecules using the green route for chemical reactions for sustainable properties.
- To inculcate the scientific temperament in the students and outside the scientific community.
- Learnt to handle sophisticated equipments for the determination and characterization of chemical compounds.
- Use of the latest chemistry software to avoid the laborious work in research.

Pedagogies used in the programme

- Conventional method such as black board and chalk, and modern methods like power point presentation and information and communications technology (ICT) are used in class room teaching.
- Molecular models are used to teach molecular symmetry, stereochemistry and solid state chemistry courses.
- Each student performs experiments as per the protocol in practical classes.
- For the preparation of new compounds, each student can adopt new experimental setup, and also exposed to different analytical instruments for qualitative and quantitative analyses. In addition to this, students will acquire skill to handle various instruments independently.
- Students will be presenting seminars in each semester.
- Each student will be subjected to viva-voce examinations in every semester.
- Every student will work for project on a small research problem.
- Rigorous training will be giving for every student to interpret spectral data in the respective course including their dissertation.
- Special lectures are delivered by eminent scholars from different intuitions.
- National/International conferences are organized to upgrade the subject knowledge.

GENERAL REQUIREMENTS

Scheme of instructions

1. A Masters Degree programme 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.

2. 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 Hardcore, Soft Core and Open Elective. A candidate may earn another 04 credits by studying MOOCs/SWAYAM courses.

3. **Minimum for Pass:** In case a candidate secures less than 30% in C_1 and C_2 put together, the candidate is said to have DROPPED the course, and such a candidate is not allowed to appear for C_3.

4. In case a candidate secures less than 30% in C_3, or secures more than 30% in C_3 but less than 50% in C_1, C_2 and C_3 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.

5. **Credits (Minimum) Matrix:** A candidate has to study 48 credits from hard Core, a minimum of 34 credits in Soft Core (sum total of 4 semesters) and 04 credits in Open Elective (II or III Semester) for the successful completion of the Masters Degree programme.

6. All other rules and regulations hold good which are governed by the University of Mysore from time to time.

Definitions

1. In the Choice Based Credit System – Continuous Assessment Grading Pattern (CBCS-CAGP), programme means a course and a course means a paper.
2. **HC:** Hard Core; **SC:** Soft Core; **OE:** Open Elective

GENERAL SCHEME WITH RESPECT TO ASSESSMENT OF CREDITS

Semester	Hard Core		Soft Core			Open Elective
	Theory			Theory	Practicals	
I	I	3 + 0 + 0 = 3	A	2 + 0 + 0 = 2*	0 + 0 + 4 = 4[a]	-
	O	3 + 0 + 0 = 3	I	2 + 0 + 0 = 2*	0 + 0 + 4 = 4[a]	
	P	3 + 0 + 0 = 3	O	2 + 0 + 0 = 2*	0 + 0 + 4 = 4[a]	
	A	3 + 0 + 0 = 3	P	2 + 0 + 0 = 2*	0 + 0 + 4 = 4[a]	
II	I	3 + 0 + 0 = 3	A	2 + 0 + 0 = 2*	0 + 0 + 4 = 4[a]	4 + 0 + 0 = 4[c]
	O	3 + 0 + 0 = 3	I	2 + 0 + 0 = 2*	0 + 0 + 4 = 4[a]	
	P	3 + 0 + 0 = 3	O	2 + 0 + 0 = 2*	0 + 0 + 4 = 4[a]	
	G	3 + 0 + 0 = 3	P	2 + 0 + 0 = 2*	0 + 0 + 4 = 4[a]	
III	I	3 + 0 + 0 = 3	A	2 + 0 + 0 = 2	0 + 0 + 2 = 2[ab]	4 + 0 + 0 = 4[c]
	O	3 + 0 + 0 = 3	I	2 + 0 + 0 = 2	0 + 0 + 2 = 2[ab]	
	P	3 + 0 + 0 = 3	O	2 + 0 + 0 = 2	0 + 0 + 2 = 2[ab]	
	G	3 + 0 + 0 = 3	P	2 + 0 + 0 = 2	0 + 0 + 2 = 2[ab]	
IV	I	3 + 0 + 0 = 3	A	2 + 0 + 0 = 2	0 + 0 + 2 = 2[ab]	-
	O	3 + 0 + 0 = 3	I	2 + 0 + 0 = 2	0 + 0 + 2 = 2[ab]	
	P	3 + 0 + 0 = 3	O	2 + 0 + 0 = 2	0 + 0 + 2 = 2[ab]	
	A	3 + 0 + 0 = 3	P	2 + 0 + 0 = 2	0 + 0 + 2 = 2[ab]	
Total Credits	**48**		**24 (48)**			**04**

NOTE

A–Analytical; I–Inorganic; O–Organic; P–Physical; G - Spectroscopy; (L+T+P) - Theory + Tutorial + Practical

*Courses are compulsory for chemistry students in first and second semesters.

[a] 50% of the students will attend Analytical/Inorganic Practicals and remaining 50% students will attend Organic/Physical Practicals in I or III Semesters and vice-versa during II or IV Semesters.

[b] Practicals are only for Chemistry students which are compulsory papers.

[C] Courses are common for both II and III Semesters and the candidate can opt either in II or III semester

SCHEME OF STUDY AND EXAMINATION
FIRST SEMESTER

HARD CORE THEORY

Courses	Title	Contact Hours/ week	Credit	Max. Marks	Internal Assessment Marks		Semester End Exams (C_3)	
					C_1	C_2	Duration (Hrs)	Marks
CHI HCT: 1.1	Concepts and Models of Inorganic Chemistry	3	3	100	15	15	03	70
CHO HCT: 1.2	Stereochemistry and Reaction Mechanism	3	3	100	15	15	03	70
CHP HCT: 1.3	Basic Physical Chemistry	3	3	100	15	15	03	70
CHA HCT: 1.4	Analytical data assessment and Titrimetric analysis	3	3	100	15	15	03	70

SOFT CORE THEORY

Courses	Title	Contact Hours/ week	Credit	Max. Marks	Internal Assessment Marks		Semester End Exams (C_3)	
					C_1	C_2	Duration (Hrs)	Marks
CHA SCT: 1.1/2.1	Analytical separations	2	2	100	15	15	3	70
CHI SCT: 1.2/2.2	Chemistry of Selected Elements	2	2	100	15	15	3	70
CHO SCT: 1.3/2.3	Chemistry of Natural Products-I	2	2	100	15	15	3	70
CHP SCT: 1.4/2.4	Biophysical Chemistry	2	2	100	15	15	3	70

PRACTICALS

Courses	Title	Contact Hours/ week	Credit	Max. Marks	Internal Assessment Marks		Semester End Exams (C_3)	
					C_1	C_2	Duration (Hrs)	Marks
CHA SCP: 1.1/2.1	Analytical Practicals - I	8	4	100	15	15	6	70
CHI SCP: 1.2/2.2	Inorganic Practicals - I	8	4	100	15	15	6	70
CHO SCP: 1.3/2.3	Organic Practicals - I	8	4	100	15	15	6	70
CHP SCP: 1.4/2.4	Physical Practicals - I	8	4	100	15	15	6	70

NOTE: 50% of students will attend Analytical and Inorganic Practicals and the remaining 50% of students will attend Organic and Physical Practicals in I Semester and vice-versa in II Semester.

SECOND SEMESTER

HARD CORE THEORY

Courses	Title	Contact Hours/ week	Credit	Max. Marks	Internal Assessment Marks		Semester End Exams (C_3)	
					C_1	C_2	Duration (Hrs)	Marks
CHI HCT: 2.1	Coordination Chemistry	3	3	100	15	15	03	70
CHO HCT: 2.2	Synthetic Organic Chemistry	3	3	100	15	15	03	70
CHP HCT: 2.3	Principles of Physical Chemistry	3	3	100	15	15	03	70
CHG HCT: 2.4	Molecular Symmetry and Spectroscopy	3	3	100	15	15	03	70

NOTE

Soft Core Theory: All courses are same as that described in first semester.
Practicals: Same as that of I Semester. Students who have conducted Analytical and Inorganic or Organic and Physical Practicals in the I Semester will get interchanged during II Semester.

OPEN ELECTIVE (for Non-Chemistry Students only)

Courses	Title	Contact Hours/ week	Credit	Max. Marks	Internal Assessment Marks		Semester End Exams (C_3)	
					C_1	C_2	Duration (Hrs)	Marks
CH OET: 2.1/3.1	General Chemistry	4	4	100	15	15	03	70

NOTE: The students can study this course either in II or III Semester

THIRD SEMESTER

HARD CORE THEORY

Courses	Title	Contact Hours/ week	Credit	Max. Marks	Internal Assessment Marks		Semester End Exams (C_3)	
					C_1	C_2	Duration (Hrs)	Marks
CHI HCT: 3.1	Advanced Inorganic Chemistry	3	3	100	15	15	03	70
CHO HCT: 3.2	Organometallic and Photochemistry	3	3	100	15	15	03	70
CHP HCT: 3.3	Advanced Physical Chemistry	3	3	100	15	15	03	70
CHA HCT: 3.4	Chemical Spectroscopy	3	3	100	15	15	03	70

SOFT CORE THEORY

Courses	Title	Contact Hours/ week	Credit	Max. Marks	Internal Assessment Marks		Semester End Exams (C_3)	
					C_1	C_2	Duration (Hrs)	Marks
CHA SCT: 3.1	Electrochemical methods of chemical analysis	2	2	100	15	15	3	70
CHI SCT: 3.2	Frontiers in Inorganic Chemistry	2	2	100	15	15	3	70
CHO SCT: 3.3	Chemistry of Natural Products-II	2	2	100	15	15	3	70
CHP SCT: 3.4	Materials Chemistry	2	2	100	15	15	3	70

PRACTICALS

Courses	Title	Contact Hours/ week	Credit	Max. Marks	Internal Assessment Marks		Semester End Exams (C_3)	
					C_1	C_2	Duration (Hrs)	Marks
CHA SCP: 3.1/4.1	Analytical Practicals - II	4	2	100	15	15	6	70
CHI SCP: 3.2/4.2	Inorganic Practicals – II	4	2	100	15	15	6	70
CHO SCP: 3.3/4.3	Organic Practicals – II	4	2	100	15	15	6	70
CHP SCP: 3.4/4.4	Physical Practicals – II	4	2	100	15	15	6	70

NOTE: 50% of students will attend Analytical and Inorganic Practicals and the remaining 50% of students will attend Organic and Physical Practicals in III Semester and vice-versa in IV Semester

OPEN ELECTIVE (for Non-Chemistry Students only)
The course is same as in II Semester

FOURTH SEMESTER

HARD CORE THEORY

Courses	Title	Contact Hours/ week	Credit	Max. Marks	Internal Assessment Marks		Semester End Exams (C_3)	
					C_1	C_2	Duration (Hrs)	Marks
CHI HCT: 4.1	Bioinorganic Chemistry	3	3	100	15	15	03	70
CHO HCT: 4.2	Heterocyclic and Bioorganic Chemistry	3	3	100	15	15	03	70
CHP HCT: 4.3	Nuclear, Radiation and Photochemistry	3	3	100	15	15	03	70
CHA HCT: 4.4	Optical, Thermal and Kinetic Methods of Analysis	3	3	100	15	15	03	70

SOFT CORE THEORY

Courses	Title	Contact Hours/ week	Credit	Max. Marks	Internal Assessment Marks		Semester End Exams (C_3)	
					C_1	C_2	Duration (Hrs)	Marks
CHA SCT: 4.1	Automated and methods of chemical analysis	2	2	100	15	15	3	70
CHI SCT: 4.2	Bioinorganic Photochemistry	2	2	100	15	15	3	70
CHO SCT: 4.3	Medicinal Chemistry	2	2	100	15	15	3	70
CHP SCT: 4.4	Quantum Chemistry and Biosensors	2	2	100	15	15	3	70

NOTE

Practicals: Same as that of III Semester. Students who have conducted Analytical and Inorganic or Organic and Physical Practicals in the III Semester will get interchanged during IV Semester

SCHEME OF EXAMINATION FOR C_1, C_2 AND C_3 COMPONENTS

Preamble

In view of the CBCS syllabus, following is the model distribution of marks for C_1, C_2 and C_3 Components. At a glance, the model includes HC, SC and OE courses for the assessment of marks.

The following is the scheme which will be followed for the assessment of marks for HC, SC and OE courses irrespective of the credits associated with each course. 30% of the marks will be assessed for internals (C_1 and C_2) and remaining 70% will be for the Semester end Examinations (C_3). Each course carries 100 marks and hence 30 marks will be allotted to internals and remaining 70 marks will be for Semester end Examinations. Out of 30 marks for internals, 15 marks will be allotted to each C_1 and C_2 components.

Each course (HC/SC/OE) consists of three components namely C_1, C_2 and C_3. C_1 and C_2 are designated as Internal Assessment (IA) and C_3 as Semester end Examination. Each course (HC/SC/OE) carries **100 Marks** and hence the allotment of marks to C_1, C_2 and C_3 Components will be 15, 15 and 70 marks, respectively. i.e.,

C_1 Component	15 Marks	Assessment Marks
C_2 Component	15 Marks	
C_3 Component	70 Marks	Semester end Examination
Total	**100 Marks**	

The above Scheme will be followed for all the HC, SC and OE courses in all the four semesters.

1. HARD CORE (03 CREDIT COURSES)

1.1. Distribution of Marks for C_1 and C_2 Components

Assessment Marks (C_1 + C_2) consists of 30 marks. 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 C_1 and 16th week of the semester for C_2. Home Assignment will be considered for C_1 Component and Seminar for C_2 Component only. Hence, a teacher from each unit of a course may be given 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 C_1 and C_2 is as follows: Out of 15 Marks for C_1, Internal test will be conducted for 30 Marks (10 Marks from each unit and 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). Assessment Marks for C_2 will be distributed as follows: Internal test will be conducted for 30 Marks (10 Marks from each unit and reduced to 10 Marks) and Seminar will be assessed for 20 Marks and finally its 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 5 Marks**	Seminar	20 Marks (05+05+05+05) **5 Marks will be distributed to each HC course**
Total	**15 Marks**	**Total**	**15 Marks**

1.2. Distribution of Marks for C_3 Component (Semester end Examination)

The question paper is of 3 hrs duration with the Maximum of 70 Marks. The following question paper pattern will be followed for all the theory courses (HC/SC/OE). Question paper will have FIVE main questions. All the questions will cover all the units of the course with equal marks distribution. Q. No. 1 is of Medium/ Short Answer Type questions which will have nine questions and each question carries two marks. A student has to answer any seven questions. Q. No. 2 to 5 carries 14 marks each and a student has to answer all the four questions (*No Choice*). Each main question will have three sub-sections a, b, c. An examiner may set the questions like (4+4+6) or (4+5+5) or as his/her wish. However, sub-section 'c' will have an internal choice. i.e.,

Model Question Paper Pattern

Max. Duration: 3 Hr **Max. Marks: 70**

Note: *Answer all the questions. Each question carries 14 marks.*
***Q. No*. 1**: Nine Medium/ Short Answer Type Questions and any seven should be answered. Each question carries <u>TWO marks.</u> **(7 × 2 = 14)**

***Q. No*. 2 to 5:** All the four questions have to be answered (*No Choice*). Each question carries **FOURTEEN** marks. An examiner may set the questions like (4+4+6) or (4+5+5) or as his/her wish. However, sub-section c will have an internal choice. (*Two marks questions shall be avoided for 2 to 5*). **(4 × 14 = 56)**

a)
b)
c) **OR** c)

2. SOFT CORE (02 CREDIT COURSES)

2.1. Distribution of Marks for C_1 and C_2 Components

Assessment Marks (C_1 + C_2) consists of 30 marks. It will be divided into two parts viz., ***Internal Test and Home Assignment***. Internal tests will be conducted during the 8^{th} week of the semester for C_1 and 16^{th} week of the semester for C_2. 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 C_1 and C_2 is as follows: Out of 15 Marks for IA, Internal tests will be conducted for 20 marks and reduced to 10 marks, whereas Home Assignment is for 05 Marks. i.e.,

C_1		**C_2**	
Internal Test	20 Marks (10+10) **Reduced to 10**	Internal Test	20 Marks (10+10) **Reduced to 10**
Home Assignment	10 Marks (05+05) **Reduced to 05**	Home Assignment	10 Marks (05+05) **Reduced to 05**
Total	**15 Marks**	**Total**	**15 Marks**

2.2. Distribution of Marks for C_3 Component (Semester End Examination)

The above described pattern (1.2) holds good in this case also.

3. PRACTICALS

The following Scheme will be applicable for all the four semesters (SC for chemistry students only)

Each practical consists of three components namely C_1, C_2 and C_3. C_1 and C_2 are designated as Internal Assessment (IA) and C_3 as Semester End Examination. Each practical carries **100 Marks** and hence the allotment of marks to C_1, C_2 and C_3 Components will be 15, 15 and 70 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**	

3.1. Distribution of Marks for C_1 and C_2 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, 05 marks are allotted for Continuous Assessment. Internal tests will be conducted for 05 Marks during the 8^{th} week of the semester for C_1 and 16^{th} week of the semester for C_2. Finally, remaining 05 Marks will be for the record. i.e.,

C_1		**C_2**	
Internal Test	05 Marks	Internal Test	05 Marks
Continuous Assessment	05 Marks	Continuous Assessment	05 Marks
Record	05 Marks	Record	05 Marks
Total	**15 Marks**	**Total**	**15 Marks**

3.2. Distribution of Marks for C_3 Component (Semester End Examination)

The end examination will be conducted for **70 Marks/course** with a maximum duration of 6 hours. Two experiments will be given to each student which carries 30 Marks each. Each student will be subjected to Viva-Voce Examination for which 10 Marks is allotted. i.e.,

Two Experiments	30+30 Marks
Viva-Voce	10 Marks
Total	**70 Marks**

Note: Examiners have to set at least one experiment from each part in the semester end Examination (C_3).

FIRST SEMESTER

CHI HCT: 1.1. CONCEPT AND MODELS OF INORGANIC CHEMISTRY

Objectives:

- To study the structures of ionic crystals and simple molecules through VSEPR model.
- To learn acid-base concepts and chemical reactions in non-aqueous, ionic liquids and supercritical fluids as media.
- To study the chemistry of f-block elements.

Course outcome:

- The periodic properties of the elements, structures of ionic solids and their lattice energy calculations. Further, the use of VSEPR concepts in analyzing the structures of simple molecules.
- Various acid-base concepts and their applications in different fields. Also, understand the utility of various non-aqueous solvents in inorganic synthesis.
- Complete understanding of the chemistry of lanthanides, actinides and their applications.

Pedagogy:

- Familiarize the students with the periodic properties of the elements using modern periodic table.
- Teaching through conventional method such as black board and chalk, and modern methods like power point presentation.
- For teaching structures of solids, crystal models (MX and MX2 types) are used.

Course content

UNIT-I

[16 HOURS]

Chemical Periodicity: Review of periodic properties

Structures and energetics of ionic crystals: Introduction, MX (NaCl, CsCl, ZnS) and MX_2 (fluorite, rutile, β-crystobalite, cadmium chloride and cadmium iodide) types. The perovskite and spinel structures. Thermodynamics of ionic crystal formation. Hydration energy and solubility of ionic compounds, Lattice energy, Born-Haber cycle, Born-Lande equation.The Kapustinskii's equation, Consequences of lattice enthalpies.Applications of lattice energetics. Ionic radii, factors affecting the ionic radii, radius ratio rules.

Structures and energetics of inorganic molecules: Introduction, Bent's rule, Energetics of hybridization. VSEPR model for explaining structure of molecules including fluxional molecule. M.O. treatment of homo-nuclear and heteronuclear diatomic molecules. M.O. treatment involving delocalized π-bonding (CO_3^{2-}, NO_3^-, NO_2^-, CO_2 and N_3^-), M.O. correlation diagrams (Walsh) for triatomic molecules.

UNIT-II

[16 HOURS]

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.

Non-aqueous solvents: Classification of solvents, Properties of solvents (dielectric constant, donor and acceptor properties) protic solvents (anhydrous H_2SO_4, HF and glacial acetic acid)

aprotic solvents (liquid SO_2, BrF_3 and N_2O_4). Solutions of metals in liquid ammonia, hydrated electron. Super acids and super bases. Heterogeneous acid-base reactions.
Ionic liquids: Molten salt solvent systems, Ionic liquids at ambient temperature, Reactions in and applications of molten salt/ionic liquid media.
Supercritical fluids: Properties of supercritical fluids and their uses as solvents. Supercritical fluids as media for inorganic chemistry

UNIT-III

[16 HOURS]

Lanthanoid chemistry: General trends, Electronic, optical and magnetic properties. Abundance and extraction, **General principles**: conventional, solvent extraction and ion-exchange methods. Separation from monazite. Chemistry of principal oxidation states (II, III and IV). Stability of tetrahalides, dihalides and aqua ions of simple lanthanide compounds. Redox potentials.**Uses:** lanthanides as shift reagents, lanthanides as probes in biological systems. High temperature super conductors.
Actinoid chemistry: General trends and electronic spectra**.** Occurrence and preparation of elements, **Isolation of the elements**: thorium and uranium, enrichment of uranium for nuclear fuel, uranium hydrides, oxides and chlorides. Chemical reactivity and trend. Chemistry of trans-uranium elements.
Supramolecular Chemistry: Introduction, selectivity and Supramolecular Interactions.

References

1. Basic Inorganic Chemistry – 3rd edition. F.A. Cotton, G. Wilkinson and P.L. Gaus, John Wiley and Sons (2002).
2. Inorganic Chemistry, 3rd edition. James E. Huheey, Harper and Row Publishers (1983).
3. Inorganic Chemistry, 5th edition. G.L. Miessler, P. J. Fischer and D.A. Tarr, Pearson (2014).
4. Inorganic Chemistry, 6th edition. D.F. Shriver, M. Weller. T. Overton, J. Rourke and F. Armastrong, Oxford University Press (2014).
5. Inorganic Chemistry, 4th edition. C.E. Housecroft and A.G. Sharpe, Pearson Education Ltd. (2012).
6. Introduction to Modern Inorganic Chemistry, K.M. Mackay and R.A. Mackay, Blackie Publication (1989).
7. Concepts and Models of Inorganic Chemistry 3rd edition. B.E. Douglas, D.H. McDaniel and Alexander, Wiley (2001).
8. Ionic liquids-Classes and Properties (Ed) by Scott T. Handy, Intech Publisher (2011).
9. Lanthanide and Actinide Chemistry, Simon Cotton, John Wiley and Sons Ltd., (2006).
10. Supramolecular Chemistry, Peter J. Cragg, Springer (2010).

CHO HCT: 1.2. STEREOCHEMISTRY AND REACTION MECHANISM

Objectives:

- To understand detailed molecular structures of organic compounds.
- To learn bonding and chemical reactions of organic compounds.
- To study different chemical reactions involved in organic synthesis.

Course outcome:

- Optical and geometrical isomerism of Organic compounds. Application of stereochemistry in the study of regioselective and regiospecific reactions.
- The study of HMOT and its applications to simple organic molecules, and also understand the concept of aromaticity and methods of determining reaction mechanism.
- Nucleophilic, electrophilic and elimination reactions.

Pedagogy:

- Molecular models are used to teach stereochemistry.
- Teaching through conventional method such as black board and chalk, and modern methods like power point presentation.

Course content

UNIT-I

[16 HOURS]

Stereoisomerism: Projection formulae [flywedge, Fischer, Newman and sawhorse], enantiomers, diastereoisomers, mesomers, racemic mixture and their resolution, configurational notations of simple molecules, DL and RS configurational notations.

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

Stereoselectivity: Meaning and examples of stereospecific reactions, stereoselective reactions, diastereoselective reactions, regioselective, regiospecific reactions, enantioselective reactions and enantiospecific reactions.

UNIT-II

[16 HOURS]

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

Bonding in organic systems: Theories of bonding-molecular orbital approaches. Huckel molecular orbital theory and its application to simple π-systems: ethylene, allyl, cyclopropyl, butadienyl, cyclopentadienyl, pentadienyl, hexatrienyl, cyclohexatrienyl, heptatrienyl, cycloheptatrienyl systems. Calculation of the total π-energy, and M.O. coefficients of the systems.

Aromaticity: Concept of aromaticity, Huckel's rule, Polygon rule, annulenes, heteroannulenes and polycyclic systems.

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. Identification of products. Determination of reaction intermediates, isotope labeling and effects of cross over experiments. Kinetic and stereochemical evidence, solvent effect. Formation, structure, stability, detection and reactions of carbocations (classical and non-classical), carbanions, free radicals, carbenes, nitrenes, arynes and ylides (Sulphur, nitrogen and phosphorous).

UNIT-III

[16 HOURS]

Aliphatic Nuleophilic Substitution reactions: Kinetics, mechanism and stereochemical factor affecting the rate of S_N^1, S_N^2, S_{RN}^i, S_N^i, $S_N^{1\prime}$, $S_N^{2\prime}$, S_N^{1i} and S_{RN}^1 reactions, Neighbouring group participation.

Electrophilic substitution reactions: Kinetics, mechanism and stereochemical factor affecting the rate of S_E^1 & S_E^2

Aromatic electrophilic substitution reactions: Mechanism of nitration, halogenation, sulphonation, Friedel-Crafts alkylation and acylation, Mannich reaction, chloromethylation, Vilsmeier Haack reaction, Diazonium coupling, Gattermann–Koch reaction, Mercuration reaction.

Aromatic nucleophilic substitution reactions: S_N^1, S_N^2 and benzyne mechanism, Bucherer reaction, von Richter reaction.

Mechanism of Addition reactions: Addition to C=C multiple bonds involving electrophiles, nucleophiles. Markownikoff's rule and anti-Markownikoff's rule.

Additions to carbonyl compounds: Addition of water, alcohol, bisulphate, HCN and amino compounds. Hydrolysis of esters.

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

References

1. Stereochemistry of carbon compounds, Ernest L. Eliel.
2. Stereochemistry: P. S. Kalsi.
3. Organic Chemistry, VI edition, Robert T. Morrison, Robert N. Boyd.
4. Organic Chemistry, Vol-I by I. L. Finar.
5. Advance Organic Chemistry, IV edition, Jerry March.
6. Advance Organic Chemistry, III edition, Part-A and Part-B, Francis A. Carey and Rechard J. Sundberg.
7. Organic Chemistry, III edition, V. K. Ahluwalia and Rakesh Kumar Parashar.
8. Reactive intermediates in Organic Chemistry, N. S. Isaacs.

CHP HCT: 1.3. BASIC PHYSICAL CHEMISTRY

Objectives:

- To understand thermal properties of chemical compounds.
- To study the rate of chemical reactions including fast reactions and factors influencing the reaction rate.
- To understand the theory of electrochemistry in solution.

Course outcome:

- The completion of this course will enable the students to gain the knowledge on fundamentals and theoretical background on the concepts of chemical thermodynamics, chemical kinetics and electrochemistry of solutions.
- This helps in understanding the stability and energetics of reaction.

Pedagogy:

- Teaching through conventional method such as black board and chalk, and modern methods like power point presentation.
- To teach electrochemical aspects through animations.

Course content

UNIT-I

[16 HOURS]

Chemical Thermodynamics: Entropy: Physical significance, entropy changes in an ideal gas. Variation of entropy with temperature, pressure and volume. Entropy changes in reversible and irreversible processes.

Free energy: Helmholtz and Gibbs free energies, Gibbs-Helmholtz equation and its applications, Maxwell's relations and its applications. Nernst heat theorem: its consequences and applications. Third law of thermodynamics: statements, applications and comparison with Nernst heat theorem.

Partial molar properties: Physical significance, determination of partial molar volumes by intercept method and from 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: Relation between fugacity and pressure, variation of fugacity with temperature and pressure. Determination of fugacity of gases.

Activity and activity coefficient: Variation of activity with temperature and pressure. Determination of activity co-efficient by vapour pressure, depression in freezing point, solubility measurements and by electrical methods.

Thermodynamics of dilute solutions: Raoult's law, Henry's law. Ideal and non-ideal solutions.

UNIT-II

[16 HOURS]

Chemical Kinetics: Complex reactions: Kinetics of parallel, consecutive and reversible reactions. Chain reactions: Branched chain reactions, general rate expression, Auto catalytic reactions (Hydrogen-Oxygen reaction), oscillatory reactions and explosion limits.

Theories of reaction rates: Collision theory and its limitations, Activated complex theory (postulates -derivation) and its applications to reactions in solution. Energy of activation, other activation parameters - determinations and their significance. Lindemann theory, Hinshelwood's theory of unimolecular reactions.

Potential energy surfaces: Features and construction, theoretical calculations of E_a.

Reactions in solution: Ionic reactions - salt effects, effect of dielectric constant (single and double sphere models). Effect of pressure, volume and entropy change on the rates of reactions. Cage effect with an example.

Fast reactions- Introduction, study of fast reactions by continuous and stopped flow techniques, relaxation methods (T-jump and P-jump methods), flash photolysis, pulse and shock tube methods.

UNIT-III

[16 HOURS]

Electrochemistry of solutions: Factor effecting electrolytic conductance. Debye-Huckel theory - Concept of ionic atmosphere. Debye-Huckel-Onsager equation of conductivity and its validity. 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). Transference number: True and apparent transference numbers, Abnormal transference numbers, effect of temperature on transference numbers. 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).

Irreversible electrode process: Introduction, reversible and irreversible electrodes, reversible and irreversible cells. Polarization, over voltage - concentration over voltage, activation over voltage and ohmic over voltage. Experimental determination of over voltage. Equations for concentration over potential, stationary and non-stationary surface. Butler-Volmer equation, Tafel equation. Hydrogen oxygen over voltage. Effect of temperature, current density and *p*H on over voltage. Polarography- Half wave potential, application in qualitative and quantitative analysis.

References

1. Thermodynamics for Chemists by S. Glasstone, Affiliated East-West Press, New Delhi, (1965).
2. Physical Chemistry by P.W. Atkins, ELBS, 5th edition, Oxford University Press (1995).
3. Text Book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2nd edition (1974).
4. Elements of Physical Chemistry by Lewis and Glasstone, 2nd Edn. Macmillan & Co Ltd., New York.
5. Chemical Kinetics by K.J. Laidler, Tata McGraw-Hill Pub, Co Ltd, New Delhi.
6. Chemical Kinetics by Frost and Pearson.
7. Kinetics and Mechanism of Chemical Transformation by J. Rajaram and J.C. Kuriacose, Macmillan, New Delhi.
8. Chemical Kinetics by L.K. Jain.
9. Introduction to Electrochemistry by S. Glasstone, Affiliated East-West Press, New Delhi,
10. Electrochemistry –Principles and Applications by E.G. Potter, Cleaver-Hume press Ltd, London.
11. Modern Electrochemistry Vol. I and II by J.O.M. Bockris and A.K.N. Reddy, Pentium Press, New York (1970).

CHA HCT: 1.4. ANALYTICAL DATA ASSESSMENT AND TITRIMETRIC ANALYSIS

Objectives:

- To familiarize statistical methods to validate analytical methods.
- To learn sampling techniques and conventional volumetric methods.

Course outcome:

- To enhance the skills on sampling, purification, characterizations and data analysis using instrumental techniques.
- Build a foundation of chemical principles for understanding the chemical constituents in samples.

- To understand the basic Principle of Instrumentation and analytical applications.

Pedagogy:

- Teaching through conventional method such as black board and chalk, and modern methods like power point presentation.
- To evaluate validation parameters, MS-Office tools *viz.,* MS-Excel sheets can be used.

Course content

UNIT-I

[16 HOURS]

Analytical chemistry: Its functions and applications; analytical problems and procedures, analytical techniques and methods, method validation.
Calibration and standards: Calibration, chemical standard and reference material.
Quality in analytical laboratories: quality control, quality assurance and accreditation system.
Errors in analytical measurements: measurement errors, absolute and relative errors, determinate and indeterminate errors and accumulated errors-sources, effects on results and control.
Assessment of accuracy and precision: Accuracy and precision, standard deviation, relative standard deviation, pooled standard deviation, variance, overall precision, and confidence interval.
Significance testing: Significance tests- Outlier, Q-test, F-test, t-test, and analysis of variance (ANOVA). Significant numbers.
Calibration and linear regression: Calibration, linear regression, standard addition, internal standardisation, internal normalization, external standardisation.
Figures of merit of Analytical methods: sensitivity and detection limit, linear dynamic range.
Quality control and chemometrics: Control charts, collaborative testing and multivariate statistics.

UNIT-II

[16 HOURS]

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. Insitu 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 *p*H 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.

UNIT-III

[16 HOURS]

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, Volhard, Mohr and 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.

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. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993 prenticeHall, Inc. New Delhi.
6. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders CollegePublishing, California, 1990.
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.

CHA SCP: 1.1/2.1. ANALYTICAL CHEMISTRY PRACTICALS-I

[128 HOURS]

Objectives:

- To understand basic concepts by carrying out analytical experiments.
- The experimental results are subjected to validation of analytical parameters.

Course outcome:

- Develop the skill to carry out acid-base titrimetric analysis, potentiometric and conductometric methods.
- Understand the chemistry of different chemical reactions involved in the determination of pharmaceutical, industrial and vegetable samples.

Pedagogy:

- Computer aided applications for the evaluation of experimental results.
- Each student performs experiments as per the protocol in practical classes.

Course experiments

PART-A

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 *p*H-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 *p*H of hair shampoos and *p*H determination of an unknown soda ash.
12. Analysis of water/waste water for acidity by visual, *p*H metric and conductometric titrations.
13. Analysis of water/waste water for alkalinity by visual, *p*H metric and conductometric titrations.
14. Determination of carbonate and hydroxide-analysis of a commercial washing soda by visual and *p*H-titrimetry.
15. Determination of ammonia in house-hold cleaners by visual and conductometric titration.
16. Potentiometric determination of the equivalent weight and Ka 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 *p*Ka of an acid-base indicator.

PART-B

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 KBrO3 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 SCP: 1.2/2.2. INORGANIC CHEMISTRY PRACTICALS – I

[128 HOURS]

Objectives:

- To understand basic concepts by carrying out different experiments.
- To develop the skill for the qualitative and quantitative analysis of various samples.

Course outcome:

- Determination of various analytes presents in different ore samples by volumetric, gravimetric and spectrophotometric methods.
- The chemistry of redox, complexometric and indirect methods
- The principle in the semi-micro analysis of an inorganic salt mixture

Pedagogy:

- Each student performs experiments as per the protocol in practical classes.
- Handling the instrument and pyrolysis for quantitative determination of analyte.

Course experiments

PART – A

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. Quantitative analysis of copper(II) and iron(II) in a mixture:
   i. Copper gravimetrically as CuSCN and
   ii. Iron volumetrically using cerium(IV) solution
9. Spectrophotometric determinations of:
   a. Titanium using hydrogen peroxide
   b. Chromium using diphenyl carbazide in industrial effluents
   c. Iron using thiocyanate/1,10-phenanthroline method in commercial samples
   d. Nickel using dimethylglyoxime in steel solution
10. Micro-titrimetric estimation of :
   a) Iron using cerium(IV)
   b) Calcium and magnesium using EDTA
11. Quantitative estimation of copper (II), calcium (II) and chloride in a mixture.
12. Circular paper chromatographic separation of: (Demonstration)
   a. Iron and nickel
   b. Copper and nickel

PART – B

Semimicro qualitative analysis of inorganic mixtures containing **TWO** anions and **TWO** cations (excluding sodium, potassium and ammonium cations) and **ONE** of the following less common cations: W, Mo, Ce, Ti, Zr, V 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 SemimicroInorganicQualitative 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 SCP: 1.3/2.3. ORGANIC CHEMISTRY PRACTICALS-I

[128 HOURS]

Objectives:

- To understand synthetic methods by carrying out different experiments.
- To develop the skill for the separation and qualitative analysis of binary mixtures of organic compounds.

Course outcome:

- Students are involved in the multi-step synthesis of different organic compounds.
- Understand the qualitative analysis of binary mixture of organic compounds through separation, identification of functional groups and preparation of solid derivatives.

Pedagogy:

- Each student performs experiments as per the protocol in practical classes.
- Experimental setup for the synthesis of organic compounds by every individual.

Course experiments

PART-A

Multistep synthesis

1. Preparation *p*-bromoaniline from acetanilide**.**
2. Preparation of *n*-butyl bromide from *n*-butyl alcohol.
3. Oxidation of cyclohexanol to adipic acid.
4. Esterification: Preparation of benzoccaine from *p*-nitrotoluene.
5. Diazotization (Sandmeyer's reaction): Preparation of *p*-chlorobenzoic acid from *p*-toluidine.
6. Preparation benzilic acid from benzoin**.**
7. Preparation of *o*-hydroxy benzophenone from phenyl benzoate *via* Fries rearrangement.
8. Preparation of benzanilide from benzophenone oxime *via* Beckmann rearrangement.
9. Preparation of benzoic acid from benzaldehyde (Cannizzaro Reaction).
10. Preparation of 2,4-dinitrophenylhydrazine from 2,4-dinitrochlorobenzene.
11. Preparation of *m*-nitrobenzoic acid from methylbenzoate.
12. Preparation of chalcone.

PART-B

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

References

1. Vogel' text book of practical organic chemistry, V edition, B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatehell.
2. Elementary practical organic chemistry, Part-I: Small scale preparations, Part-II: Qualitative organic analysis, By Arthur I, Vogel.
3. Hand book of organic analysis, H. T. Clarke and Norman Collie.
4. Experiments in Organic Chemistry, Louis F. Fieser.
5. Laboratory manual of Organic Chemistry by B. B. Dey and M. V. Sitaraman.
6. Practical Organic Chemistry by Mann F. G. and Saunders.

CHP SCP: 1.4/2.4. PHYSICAL CHEMISTRY PRACTICALS – I

[128 HOURS]

Objectives:

- To understand the rate of chemical reactions and factors influencing the reaction rate by carrying out kinetic experiments.
- To understand basic concepts of electrochemistry by carrying out experiments.

Course outcome:

- After the completion of this course, the students can able to develop the experimental skill and theoretical interpretation of experimental results of many physical chemistry experiments of chemical kinetics in solution phase, thermodynamics, electrochemistry and spectrophotometry.
- This helps in academics, research and industries.

Pedagogy:

- Each student performs experiments as per the protocol in practical classes.
- To optimize the reaction conditions for understanding the rate of chemical reactions.

Course experiments

PART - A

1. Study of kinetics of hydrolysis of methyl acetate in presence of two different concentrations of HCl/H_2SO_4 and report the relative catalytic strength.
2. Study of kinetics of reaction between $K_2S_2O_8$ and KI, first order, determination of rate constants at two different temperatures and E_a.
3. To study the kinetics of saponification of ethyl acetate by conductivity method at two different concentrations of NaOH and report the relative catalytic strength.
4. Determination of partial molar volume of salt-water system ($NaCl$-H_2O/KCl-H_2O/KNO_3-H_2O) systems.
5. To study the kinetics of reaction between acetone and iodine - determination of order of reaction with respect to iodine and acetone.
6. Study the kinetics of decomposition of diacetone alcohol by NaOH, determine the catalytic coefficient of the reaction and comparison of strength of alkali.
7. Determination of energy of activation for the bromide-bromate reaction.
8. Kinetics of reaction between sodium formate and iodine and determination of energy of activation.
9. Determination of heat of solution of organic acid (benzoic acid/salicylic acid) by variable temperature method (graphical method).
10. Determination of degree of association of benzoic acid in benzene by distribution method.
11. To determine the eutectic point of a two component system (Naphthalene-*m*-dinitrobenzene system).
12. Analysis of a binary mixture (Gylcerol & Water) by measurement of refractive index.
13. Determination of the molecular weight of a polymer material by viscosity measurements (cellulose acetate/methyl acrylate).

PART - B

1. Conductometric titration of a mixture of HCl and CH_3COOH against NaOH.
2. Conductometric titration of sodium sulphate against barium chloride.

3. pH titration of (a) HCl against NaOH (b) Copper sulphate against NaOH and (c) CH_3COOH/HCOOH against NaOH - determination of K_a.
4. Determination of equivalent conductance of weak electrolyte (CH_3COOH) at infinite dilution following Kohlrausch law.
5. Determination of dissociation constant and mean ionic activity coefficient of weak acids ($CH_3COOH/HCOOH/ClCH_2COOH$) by conductivity method.
6. Potentiometric titration of KI *vs* $KMnO_4$ solution.
7. Determination of dissociation constant of a weak acid ($CH_3COOH/HCOOH/ClCH_2COOH$) by potentiometric method.
8. Potentiometric titration of a mixture of halides (KCl+KI/KCl+KBr/KBr+KI) against $AgNO_3$.
9. To obtain the absorption spectra of coloured complexes, verification of Beer's law and estimation of metal ions in solution using a spectrophotometer.
10. Potentiometric titration of $K_2Cr_2O_7$ against FAS determination of redox potential and concentration of Fe^{2+} ions.
11. Conductometric titration of oxalic acid against NaOH and NH_4OH.
12. Coulometric titration I_2 vs $Na_2S_2O_3$.
13. Determination of acidic and basic dissociation constant and isoelectric point of an amino acid by pH metric method.
14. Kinetics of photodegradation of indigocarmine (IC) using ZnO/TiO_2 as photocatalyst and study the effect of [ZnO/TiO_2] and [IC] on the rate of photodegradation.

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.

SOFT CORE PAPERS

CHA SCT: 1.1/2.1. ANALYTICAL SEPARATIONS

Objectives:

- To understand fundamentals and applications of separation techniques.
- To learn extraction and chromatographic methods for the separation and identification of different compounds.

Course outcome:

- Devise a scheme to isolate organic acids, bases and neutral compounds through an extraction process.

- To apply methods of distillation, sublimation, chromatography, filtration (including Buchner filtration), evaporation, decantation, using magnetism, sieving and skimming to separate mixtures.
- To understand the terms filtrate, residue, filtration, sediment, decant, distil, distillate, chromatogram and solvent front.
- To know that mixtures are composed of constituents which are not combined.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animations are used in class room teaching.

Course content

UNIT-I

[16 HOURS]

Principles of chromatography- Chromatographic separations and classification of principal chromatographic separations. Chromatographic mechanisms-sorption isotherms; adsorption systems-stationary and mobile phases, partition systems-stationary and mobile phases. Characterization of solutes-distribution ratio, retention factor, retention time and retardation factor.

Sorption processes- adsorption, partition, ion- exchange and size exclusion.

Chromatographic performance- Efficiency and resolution. Peak asymmetry- kinetic and temperature effects. Isolation of separated components.

Quantitative and qualitative analyses.

Thin layer chromatography (TLC) - Principles and procedures, stationary and mobile phases, solute- detection, alternative TLC procedures and applications of TLC.

Gas chromatography (GC) - Principles and types. Mobile phases, Sample injections, columns and stationary phases. Temperature control and solute detection; thermal conductivity detector (TCD), flame ionization detector (FID), nitrogen-phosphorus detector (NPD) and electron capture detector (ECD). Instrument control and data processing. GC-procedures- temperature programming and special procedures used in GC. Quantitative and qualitative analyses.

High performance liquid chromatography(HPLC): Principles, mobile phases, solvent delivery systems, sample injection system, column and stationary phases. Solute detection -UV-visible, fluorescence, refractive index and electrochemical detectors. Instrument control and data processing. Modes of HPLC. Optimisation of separations, qualitative and quantitative analyses.

UNIT-II

[16 HOURS]

Ion-exchange chromatography (IEC): Principles, apparatus and instrumentation, and applications.

Size-exclusion chromatography (SEC): Principles, apparatus and instrumentation, and applications.

Affinity chromatography (AFC): Principles, methodology and applications.

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

Supercritical fluid extraction (SFE): Advantages, instrumentation, choice of supercritical fluids, off-line and on-line extraction, applications.

Electrophoresis (EP) and electrochromatography(EC): Principles- high performance capillary electrophoresis and capillary electrochromatography, running buffers, supporting medium, sample injection, solutes- detection, instrument control and data processing. Modes of EP and EC- capillary zone electrophoresis (CZE), micellar electrokineticchromatography (MEKC), capillary gel electrophoresis (CZE), capillary isoelectric focusing (CIEF). Capillary electrochromatography (CEC), features, basis of separations. Qualitative analysis by CE and CEC and applications.
Solvent and solid phase extraction: Extraction techniques, extraction efficiency and selectivity. Solvent extraction (SE) - Extraction of organic acids and bases, extraction of metals. Methods of extraction and applications. Solvent phase sorbents, solid phase extraction (SPE) formats. Automated solid phase extraction. Solid phase micro extraction (SPME). Applications of SPE and SPME.

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. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993 prenticeHall, Inc. New Delhi.
6. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders CollegePublishing, California, 1990.
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.

CHI SCT: 1.2/2.2. CHEMISTRY OF SELECTED ELEMENTS

Objectives:

- To learn basic chemistry of some selected group elements from periodic table.
- To understand properties of metal-metal bonding and cluster compounds.

Course outcome:

- Understand the chemistry of hydrogen and group 2 elements.
- The chemistry of pseudohalogens, interhalogens and their halogen compounds.
- The chemistry of xenon and other noble gas compounds.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animations are used in class room teaching.

Course content

UNIT-I

[16 HOURS]

Compounds of hydrogen: The hydrogen and hydride ions, Dihydrogen and hydrogen bonding. Classes of binary hydrides: Molecular hydrides, saline hydrides and metallic hydrides.
The Group 1 elements: Occurrence, extraction and uses. Simple compounds: Hydrides, halides, oxides, hydroxides, oxoacids, nitrides, solubility and hydration and solutions in liquidammonia. Coordination and organometallic compounds. Applications.
The Group 2 elements: Occurrence, extraction and uses. General properties.Halides, hydrides and salts of oxo acids. Complex ion in aqueous solution and complexes with amido and alkoxy ligands.
The Group 15 elements: Introduction, oxides and oxoacids of nitrogen and phosphorus.

UNIT-II

[16 HOURS]

The Group 17 elements: Occurrence, recovery and uses. Trends in properties and pseudohalogens. **Interhalogens**: Physical properties and structures, chemical properties, cationic interhalogens. **Compounds with oxygen**: Halogen oxides, oxoacids and oxoanions**.** Trends in rates of redox reactions and redox properties of individual oxidation states**.**
Chemistry of astatine.
The Group 18 elements: Occurrence, recovery and uses. Synthesis and structure of xenon fluorides, Reaction of xenon fluorides, xenon-oxygen compounds, Organoxenon compounds, other compounds of noble gases.
M-M bonds: Multiple metal-metal bonds.
Cluster compounds: carbonyl and carbide clusters.

References

1. Basic Inorganic Chemistry – 3rd edition. F.A. Cotton, G. Wilkinson and P.L. Gaus, John
2. Wiley and Sons (2002).
3. Inorganic Chemistry, 3rd edition. James E. Huheey, Harper and Row Publishers (1983).
4. Inorganic Chemistry, 3rd edition. G.L. Miessler and D.A. Tarr, Pearson Education (2004).
5. Inorganic Chemistry, 4th edition. C.E. Housecroft and A.G. Sharpe, Pearson Education Ltd. (2012).
6. Chemistry of the Elements – N.N. Greenwood and A. Earnshaw, Pergamon Press (1985).
7. Inorganic Chemistry, 6th edition. D.F. Shriver, M. Weller. T. Overton, J. Rourke and F. Armastrong, Oxford University Press (2014).

CHO SCT: 1.3/2.3. CHEMISTRY OF NATURAL PRODUCTS-I

Objectives:

- To learn the nomenclature, classification, purification, structure and synthesis of some natural products.
- To understand the biological functions of biomolecules.

Course outcome:

- Acquire the knowledge of chemistry of lipids, prostaglandins and terpenoids.
- Understand the biological importance of chlorophyll and porphyrins.
- Chemistry of flavonoids and isoflavonoids.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern method like power point presentation is used in class room teaching.

Course content

UNIT-I

[16 HOURS]

Lipids: Nomenclature, classification, purification, structure and synthesis of fatty acids, phospholipids, sphingolipids. Biological importance of lipids (Lecithin, sphingolipids, oils and fats).
Prostaglandins: Introduction, classification and biological importance of PG's. Constitution of PGE1. Synthesis of PGE & F series.
Terpenoids: Introduction, classification and general methods of structural elucidation. Chemistry of pinene, camphor, caryophyllene, santonin. Biosynthesis of terpenoids.

UNIT-II

[16 HOURS]

Porphyrins: Introduction, structure and biological functions of haemin. Vitamin B12: structure and as coenzyme in molecular rearrangement reactions; Chlorophyll: structure and biological importance.
Flavonoids and Isoflavonoids: Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Apigenin, Luteolin, Kaempferol, Quercetin, wedelolactone, Butein, Daidzein. Biosynthesis of flavonoids and isoflavonoids: Acetate Pathway and Shikimic acid Pathway. Biological importance of flavonoids and isoflavonoids

References

1. Organic Chemistry, VI edition, Robert T. Morrison, Robert N. Boyd.
2. Organic Chemistry, Vol-II by I. L. Finar.
3. Schaum's outline of theory and problems of Organic Chemistry, Harbert Meislich, Howard Nechamkin and Jocob Sharefkin.
4. Natural products: Their chemistry and biological significance, J. Mann, R. S. Davidson, J. B. Banthorpe and J. B. Harborne.
5. Synthetic drugs, Gurdeep R. Chatwal.
6. Heterocyclic chemistry by Achison.
7. Heterocyclic chemistry by Smith and Joule.
8. Heterocyclic chemistry by Pacquete.

CHP SCT: 1.4/2.4. BIOPHYSICAL CHEMISTRY

Objectives:

- To understand the physico-chemical principles of biological fluids.
- To learn the pharmacokinetics, pharmacodynamics, toxicokinetics of biological systems.

Course outcome:

- After the completion of this course, the students gain the knowledge on theory and principles of biophysical chemistry and pharmacokinetics.
- This course helps to understanding the bio-availability and different pharmacokinetic parameters of drugs in the living system.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animations are used in class room teaching.

Course content

UNIT-I

[16 HOURS]

Biophysical Chemistry: 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. Electro-osmosis 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 bio-membranes 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 *p*H on the viscosity of bio-molecules (albumin solution). Significance of viscosity in biological systems - mechanism of muscle contraction, 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.

UNIT-II

[16 HOURS]

Pharmacokinetics: Introduction, biopharmaceutics, pharmacokinetics, clinical pharmacokinetics, pharmacodynamics, toxicokinetics and clinical toxicology. Measurement of drug concentration in blood, plasma or serum. Plasma level-time curve, significance of measuring plasma drug concentrations.

One compartment open model: Intravenous route of administration of drug, elimination rate constant, apparent volume of distribution and significance. Calculation of elimination rate constant from urinary excretion data, clinical application.

Two compartment model: Plasma level-time curve, relationship between tissue and plasma drug concentrations, Apparent volumes of distribution. Drug clearance, clinical example. Plasma level-time curve for a three compartment open model.

Drug absorption: Factors affecting the rate of drug absorption - nature of the cell membrane, Route of drug administration - Oral drug absorption, Intravenous infusion and intravenous solutions, Effect of food on gastrointestinal drug absorption rate.

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. Applied Biopharmacokinetics and Pharmacokinetics - Leon Shargel, Andrew YuPrentice-Hall International, Inc (4th edition).

6. Essentials of Physical Chemistry and Pharmacy – H.J. Arnikar, S.S. Kadam, K.N. Gujan, Orient Longman, Bombay, (1992).

SECOND SEMESTER

CHI HCT: 2.1. COORDINATION CHEMISTRY

Objectives:

- To understand the preparation, properties, electronic configuration and structural elucidation of coordination compounds.
- To learn the reaction mechanism, stereochemistry and photochemistry of coordination compounds.

Course outcome:

- Gain the knowledge of preparative methods of coordination compounds and geometries of different coordination numbers.
- Understand the CFT and MOT bonding theories of metal complexes.
- Electronic spectra, magnetic properties and infrared spectroscopy of coordination compounds. In addition, understand the reaction mechanism and photochemistry of coordination compounds.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animations are used in class room teaching.

Course content

UNIT-I

[16 HOURS]

Preparation of coordination compounds: Introduction, Preparative methods- simple addition reactions, substitution reactions, oxidation-reduction reactions, thermal dissociation reactions. Geometries of metal complexes of higher coordination numbers (2-12).

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.

Determination of stability constants: Theoretical aspects of determination of stability constants of metal complexes by spectrophotometric 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.

Molecular Orbital Theory: MOT to octahedral, tetrahedral and square planar complexes without and with pi-bonding.

UNIT-II

[16 HOURS]

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. Charge transfer and energy applications. Optical rotatory dispersion and Circular dichroism. Magnetic circular dichroism.

Magnetic properties: Introduction, magnetic susceptibility and its measurements, spin and orbital contributions to the magnetic moment, the effects of temperature on μeff, spin-cross over, ferromagnetism, anti-ferromagnetism and ferrimagnetism.
Applications of infrared spectroscopy of coordination compounds: Metal complexes of ammine, nitro, nitrito, hydroxo, carbonato, sulphato, cyano, cyanato and thiocyanato complexes.

UNIT-III

[16 HOURS]

Reactions 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.
Stereochemistry of reactions- Substitution in *trans* and its complexes, isomerization of chelate rings. Substitution reactions of square-planar complexes-kinetics and stereochemistry of square-planar substitutions, evidence for associative reactions, explanations of the *trans* effect.
Electron-transfer processes: Inner-sphere mechanism and outer-sphere mechanism, conditions for high and low oxidation numbers.
Photochemistry of coordination compounds: Photochemistry of chromium(III) ammine compounds, Light-induced excited state spin trapping in iron(II) compounds and MLCT photochemistry in pentammineruthenium(II) compounds.

References

1. Physical Inorganic Chemistry- A Coordination Chemistry Approach- S.F.A. Kettle, Spektrum, Oxford, (1996).
2. Inorganic Chemistry-4th edition. C.E. Housecroft and A.G. Sharpe, Pearson Education Ltd. (2012).
3. Inorganic Chemistry-5th edition. G.L. Miessler, P. J. Fischer and D.A. Tarr, Pearson (2014).
4. Inorganic Chemistry-6th edition. D.F. Shriver, M. Weller. T. Overton, J. Rourke and F. Armastrong, Oxford University Press (2014).
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).
7. Infrared and Raman Spectra of Coordination Compounds, Part-B- 6th edition, K. Nakamoto, John Wiley and Sons (2009).

CHO HCT: 2.2. SYNTHETIC ORGANIC CHEMISTRY

Objectives:

- To understand the reactions of organic compounds involving various reagents.
- To learn the synthesis and retro-synthesis of different organic compounds.

Course outcome:

- Students are familiar about chemistry of oxidants, reductants and their applications in the organic synthesis.
- Understand the various catalysts in organic synthesis by known naming reactions.
- Retro-synthesis and molecular rearrangement.

Pedagogy:

- Conventional method such as black board and chalk is used.

- Modern method like power point presentation is used in class room teaching.

Course content

UNIT-I

[16 HOURS]

Oxidation: Oxidation with chromium and manganese reagents (CrO_3, $K_2Cr_2O_7$, PCC, PDC, Sarret reagent, MnO_2, $KMnO_4$, ozone, peroxides and peracids, periodic acid, OsO_4, SeO_2, NBS, Oppenauer oxidation, Sharpless epoxidation.

Reduction: Catalytic hydrogenation (homogeneous and heterogeneous) – catalysts (Pt, Pd, Ra-C, Ni, Ru, Rh), solvents and reduction of functional groups, catalytic hydrogen transfer reactions. Wilkinson catalyst, $LiAlH_4$, $NaBH_4$, DIBAL-H, Sodium cyanoborohydride, dissolving metal reactions (Birch reduction). Leukart reaction (reductive amination), diborane as reducing agent, Meerwein-Ponndorf-Verley reduction, Wolff-Kishner reduction, Clemensen reduction, tributyl tinhydride, stannous chloride, Bakers yeast, Organoboron compounds: Introduction and preparations. Hydroboration and its applications. Reactions of organoboranes: isomerization reactions, oxidation, protonolysis, carbonylation, cyanidation. Reactions with aldehydes or ketones (*E* and *Z*-alkenes).

UNIT-II

[16 HOURS]

Reagents and reactions in organic synthesis: Use of following reagents in organic synthesis and functional group transformations: Lithium diisopropylamide (LDA), Gilmann reagent, dicyclohexyl carbodimide (DCC), dichlorodicyanoquinone (DDQ), Silane reagents-trialkylsilyl halides, trimethylsilyl cyanide, trimethyl silane, phase transfer catalyst, crown ethers, cyclodextrins, Ziegler-Natta catalyst, diazomethane, Woodward and Prevost hydroxylation, Stark enamine reaction, phosphorous ylides - Wittig and related reactions, sulphur ylides – reactions with aldehydes and ketones, 1,3-dithiane anions - Umpolung reaction, Peterson reaction. Palladium reagents: Suzuki coupling, Heck reaction, Negishi reaction. Green Chemistry: Definition and principles, planning green synthesis in the laboratory, green preparations- aqueous reactions, solid state (solvent free) reactions, photochemical reactions, enzymatic transformations and reactions in ionic liquids.

UNIT-III

[16 HOURS]

Molecular rearrangements: Introduction Carbon to carbon migration: Pinacol-pinacolone, Wagner-Meerwein, Benzidine, benzylic acid, Favorskii, Fries rearrangement, dienophile rearrangement. Carbon to nitrogen migration: Hofmann, Curtius, Lossen, Schmidt and Beckmann rearrangements. Miscellaneous rearrangements: Wittig, Smiles, Bayer-Villeger rearrangement and Barton 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, tetralone, ibuprofen, functional group transformations in organic synthesis; nitro to keto, nitro to aniline, acid to alcohol etc..

References

1. Organic Chemistry, VI edition, Robert T. Morrison, Robert N. Boyd.
2. Organic Chemistry, Vol-I & II by I. L. Finar.
3. Advance Organic Chemistry, IV edition, Jerry March.

4. Advance Organic Chemistry, III edition, Part-A and Part-B, Francis A. Carey and Rechard J. Sundberg.
5. Organic Chemistry, III edition, V. K. Ahluwalia and Rakesh Kumar Parashar.
6. Organic named reactions and molecular rearrangements, Gudeep Raj.
7. Modern synthetic reactions, II edition, H. O. House.
8. Organic synthesis, Jagadamba Singh and L. D. S. Yadav.
9. Green Chemistry, K. R. Desai.
10. Principles of Organic synthesis, R. O. C. Norman and J. M. Coxon.
11. Organic synthesis II edition, V. K. Aluwalia and Renu Agarwal.
12. Organic synthesis, Robert E. Ireland.
13. Schaum's outline of theory and problems of Organic Chemistry, Harbert Meislich, Howard Nechamkin and Jocob Sharefkin.
14. Organic chemistry by Clayden, Greeves, Warren and Wothers.

CHP HCT: 2.3. PRINCIPLES OF PHYSICAL CHEMISTRY

Objectives:

- To understand the theoretical calculations of energies of simple molecules.
- To learn the calculation of different energies by statistical thermodynamics.
- To understand the basics of polymers, their kinetics and applications.

Course outcome:

- Principles of Quantum chemistry and theoretical calculations of energies of molecules and chemical reactions.
- Apply solutions of the Schrödinger equation for simple systems (particle in a box, rigid rotor, harmonic oscillator) to real systems (vibrational, rotational, and electronic energy states) in determining the energy of stationary states.
- Explain angular momentum as possessed by atomic or molecular systems, various descriptions of how angular momentum can be coupled, and how conservation of angular momentum is important to spectroscopy.
- Concepts and applicability of statistical thermodynamics in the calculations of different energies in the reacting system. Applications of phase rule for separation of the metals from ore.
- Fundamentals of polymers and their applications in controlling the quality and waste management of polymer product.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern method like power point presentation is used in class room teaching.
- Assigning the students to solve the problems to understand the concepts.

Course content

UNIT-I

[16 HOURS]

Quantum Chemistry: Introduction to quantum mechanics: Schrödinger wave equation, time-independent and time dependent Schrödinger wave equation and the relation between their solutions. Eigen functions and Eigen values. Physical interpretation of wave function. Concept of operators – Laplacian, Hamiltonian, Linear and Hermitian operators. Angular momentum operators and their properties. Commutative and non-commutative operators. Normalization, orthogonality and orthonormality of wave functions. Postulates of quantum mechanics. Solutions of Schrödinger wave equation for free particles, particle in a ring, particle in three dimensional box. Quantum mechanical degeneracy, tunnelling (no derivation). Wave equation for H-atom, separation and solution of R, ϕ and θ equations. Application of Schrodinger equation to rigid rotator and harmonic oscillator. Eigen functions and Eigen values of angular momentum. Ladder operator method for angular momentum.

UNIT-II

[16 HOURS]

Statistical thermodynamics: Objectives of statistical thermodynamics, concept of distribution, types of ensembles. Thermodynamic probability and most probable distribution law. Partition functions – definition, evaluation of translational, rotational and vibrational and electronic partition functions for monoatomic, diatomic and polyatomic gaseous molecules. Sackur-Tetrode equation for entropy of translation function. Calculation of thermodynamic functions and equilibrium constants in terms of partition functions. Different distribution laws (Types of statistics): Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac Statistics (derivation of the three distribution laws). Comparison of Bose-Einstein and Fermi-Dirac Statistics with Maxwell-Boltzmann statistics. Problems and their solutions.

Phase rule studies: Thermodynamic derivation of phase rule. Application of phase rule to the two component systems - compound formation with congruent melting point and incongruent melting points, Roozeboom's classification. Application of phase rule to three component systems- systems of three liquids and systems of two salts and water.

UNIT-III

[16 HOURS]

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 methods.

Kinetics of Polymerization - Condensation, addition, free radical, ionic, co-ordination polymerization.

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.

Colloids: Types and classification, Micelles: Surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, micellar catalysis.

References

1. Text Book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2nd edition (1974).
2. Quantum Chemistry – A.K. Chandra. 2nd edition, Tata McGraw Hill Publishing Co. Ltd., (1983).
3. Quantum Chemistry – Eyring, Walter and Kimball. John Wiley and Sons, Inc., New York.
4. Quantum Chemistry – I.N. Levine. Pearson Education, New Delhi, (2000).
5. Theoretical Chemistry – S. Glasstone. East West Press, New Delhi, (1973).

6. Quantum Chemistry – R.K. Prasad, New Age International Publishers, (1996).
7. Text Book of Polymer Science, F.W. Billmeyer, Jr., John Wiley, London (1994).
8. Polymer Science. V. R. Gowrikar, N.V. Vishwanathan and J. Sreedhar, Wiley Eastern, New Delhi (1990).
9. Fundamentals of Polymer Science and Engineering. A. Kumar and S.K. Gupta, Tata – McGraw Hill New Delhi (1978).
10. Polymer Characterization, D. Campbell and J.R. White, Chapman and Hall, New York.
11. Fundamental Principles of Polymer Materials, R.L. Rosen, John Wiley and Sons, New York.

CHG HCT: 2.4. MOLECULAR SYMMETRY AND SPECTROSCOPY

Objectives:

- To understand the concepts of symmetry and symmetry operations and their application to CFT, hybridization, MOT and vibrational spectroscopy.
- To learn the theory and applications of microwave, vibration and Raman spectroscopy.
- To understand the principles and applications of UV-Visible and resonance Raman spectroscopy.

Course outcome:

- Molecular symmetry and applications of group theory to CFT, hybridization, MOT and vibrational spectroscopy.
- Theory and principles of Rotation, Vibration and Raman Spectroscopy.
- Theory and principles Electronic and Resonance Raman spectroscopy.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Molecular models are used to teach symmetry aspects of molecules
- Modern methods like power point presentation and animations are used in class room teaching.
- Students will be assigned to solve the numerical problems.

Course content

UNIT-I

[16 HOURS]

Molecular symmetry and group theory: Symmetry elements and symmetry operations.

The Point Groups Used with Molecules: Concept of a group, definition of a point group. Classification of molecules into point groups. Subgroups.

Hermann-Maugin symbols for point groups. Multiplication tables (C_{2V}, C_{2h} and C_{3V}). Matrix notation for the symmetry elements. Classess 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}). Symmetry and dipole moment.

Applications of group theory: Group theory and hybrid orbitals.

Symmetry in Chemical bonding: Group theory to Crystal field theory and Molecular orbital theory (octahedral and tetrahedral complexes).

Symmetry in Vibrational Spectroscopy: Determining the symmetry groups of normal modes for non-linear molecules (H_2O, NH_3, CH_4, trans-N_2F_2) and linear molecules (CO, HCl, HCN and CO_2) (Integration method).

UNIT-II

[16 HOURS]

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. Classification of polyatomic molecules based on moment of inertia. Rotation spectra of polyatomic molecules (OCS CH_3F and BCl_3). 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, expressions for fundamental and overtone frequencies. Vibration - rotation spectra of carbon monoxide. Vibration of polyatomic molecules – The number of degrees of freedom of vibration. Parallel and perpendicular vibrations (CO_2 and H_2O). Combination, difference and hot bands. Fermi resonance. Force constant and its significance. Theory of infrared absorption and theoretical group frequency. Intensity of absorption band and types of absorptions. Applications: Structures of small molecules: XY_2 – linear or bent, XY_3 – planar or pyramidal.

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. Raman activity of vibrations, rule of mutual exclusion principle. Vibration modes of some simple molecules and their activity.

UNIT-III

[16 HOURS]

UV Visible spectroscopy: Quantitative aspects of absorption – Beer's law, Technology associated with absorption measurements. Limitations– real, chemical, instrumental and personal. Theory of molecular absorption. Vibration- rotation fine structure of electronic spectra. Types of absorption bands- n to π*, π to π*, n to σ* and σ to σ*, C-T and ligand field. Instrumentation.

Applications: Qualitative and quantitative analysis of binary mixtures, measurements of dissociation constants of acids and bases, determination of molecular weight. Woodwards empirical rules for predicting the wavelength of maximum absorption for olefins, conjugated dienes, cyclic trienes and polyenes, α,ß-unsaturated aldehydes and ketones, benzene and substituted benzene rings.

Resonance Raman Spectroscopy: Resonance Raman Effect and its applications. Non-linear Raman effects: Hyper, stimulated and inverse Raman effects. Coherent Anti-Stokes Raman Scattering and its applications.

References

1. Chemical Applications of Group Theory, 3rd edition, F.A. Cotton, John Wiley and
2. Sons (2006).
3. Molecular Symmetry and Group Theory – Robert L Carter, John Wiley and Sons (2005).
4. Symmetry in Chemistry - H. Jaffe and M. Orchin, John Wiley, New York (1965).
5. Molecular Symmetry – David J. Willock, John Wiley and Sons Ltd., (2009).
6. Group Theory and its Chemical Applications - P.K. Bhattacharya, HimalayaPublications, New Delhi (1998).
7. Fundamentals of Molecular Spectroscopy, C.N. Banwell and E.M. McCash. 4^{th} edition, Tata McGraw Hill, New Delhi.
8. Fundamentals of molecular spectroscopy, G. M. Barrow, MgGraw Hill, New York (International students Edition), 1974.
9. Theoretical chemistry, S. Glasstone, affiliated East-West Press Pvt. Ltd, New Delhi, 1973.
10. Spectroscopy, B.P. Straughan and S. Walker, John Wiley & Sons Inc., New York, Vol. 1 and 2, 1976.
11. Vibration Spectroscopy Theory and Applications, D.N. Satyanarayana, New Age International, New Delhi (2004).
12. Spectroscopy, B.P. Straughan and S. Salker, John Wiley and Sons Inc., New York, Vol.2, 1976.
13. Organic Spectroscopy, William Kemp, English Language Book society, Macmillan, 1987.
14. Instrumental methods of analysis, H. H. Willard, L. L. Merritt and J. A. Dean, 7^{th} Edition, 1988.
15. Physical methods in inorganic chemistry, R. S. Drago, affiliated East-West press Pvt. Ltd., (Student Edition) 1978.

OPEN ELECTIVE (FOR NON-CHEMISTRY STUDENTS ONLY)

CH OET: 2.1/3.1- GENERAL CHEMISTRY

Objectives:

- To understand the basic concepts of chemistry including periodic properties of elements, structure and bonding.
- To learn the applications of synthetic products and biological importance of natural products. .
- To understand the basic concepts of thermodynamics, chemical kinetics, ionic equilibria and electrochemistry.
- To learn the statistical evaluation of experimental data. Applications of titrimetric methods and separation techniques.

Course outcome:

- Periodic properties of elements, structure and bonding of ionic compounds as well as various concepts of acids and bases.
- Hybridization, bonding and molecular structure of simple organic molecules. And also, biological importance of natural products.
- Basic concepts of thermodynamics, chemical kinetics, electrochemistry and ionic equilibria and their applications.
- Statistical evaluation of experimental data, concept of titrimetric and chromatographic methods.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animations are used in class room teaching.
- Students will be assigned to solve the numerical problems to understand the concepts.

Course content

UNIT-I

[16 HOURS]

Periodic Table and chemical Periodicity: Periodic properties of elements, State of Matter, their resources. Important periodic properties of the elements, covalent radii, ionic radii, ionization potential, electron affinity and electronegativity.

Structure and Bonding: Properties of ionic compounds, structure of crystal lattices (NaCl, CsCl, ZnS, Wurtzite and rutile), Lattice energy, Born-Haber Cycle, radius ratio rules and their limitations.MO treatment for homo- and heteronuclear diatomic molecules. VSEPR model to simple molecules. Factors affecting the radii of ions, covalent character in ionic bonds, hydration energy and solubility of ionic compounds.

Concepts of Acids and Bases: Review of acid base concepts**.** Lux-Flood and solvent system concepts. Hard-soft acids and bases. Applications.

UNIT-II

[16 HOURS]

Bonding and molecular structure: Introduction to organic chemistry, atomic orbitals, sigma and pi bond formation-molecular orbital (MO) method, sp, sp^2 and sp^3 hybridization, bond length, bond dissociation energies and bond angles (open chain and cyclic compounds). Electronegativity and polarity of the bonds. Classifications and reactions of organic compounds (with examples).

Acids and bases: Hydrogen bonding, resonance and inductive effective on strengths of acids and bases.

Biological importance of natural products: Amino acids, proteins, carbohydrates (cellulose, starch, glycogen), lipids (fats and oils, phospholipids), prostaglandins, nucleic acids, steroids, alkaloids, vitamins, flavonoids.

Applications of synthetic products: Dyes, drugs, polymers (plastics), soaps and detergents, pesticides and pheromones.

UNIT-III

[16 HOURS]

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.

Chemical kinetics: Rate and order of reaction. Factor affecting the rate of reaction. and determination Order of reaction. Energy of activation and its determination. Brief account of collision and activated complex theories.

Ionic equilibria: pH scale, buffer solutions, calculation of pH of buffer solutions, buffer capacity and buffer index, buffer mixtures.

Solutions: Concentration units, solutions of liquids in liquids, Raoult's law, ideal and non-ideal solutions.

Electrochemistry: Electrolytic conductance, specific, equivalent and molar conductance, ionic mobility and transference number, factors affecting the electrolytic conductance, Arrhenius theory of strong and weak electrolytes, assumptions of Debye-Huckel theory of strong electrolytes. Single electrode potential, reference electrodes, galvanic cells, emf of galvanic cells and construction of electrochemical cells.

UNIT-IV

[16 HOURS]

Basic Statistics and Data Handling: Significant figures, accuracy and precision. Types of errors: Determinate error and indeterminate error. Definitions for statistics. Quantifying random error: Confidence limits, variance. Rejection of results.

Applications of titrimetric methods: Introduction, theory and applications of acid base titrimetry, complexometric titrations and redox titrimetry

Separation techniques: Purification-Crystallization, sublimation, fractional crystallization, distillation techniques (simple distillation, steam distillation, distillation under reduced pressure, and fractional distillation), solvent extraction.

Chromatography: Thin layer chromatography and ion-exchange chromatography and their applications in the separation of the components from the mixture.

References

1. Text Book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2nd edition (1974).
2. Elements of Physical Chemistry by Lewis and Glasstone, 2nd Edn. Macmillan & Co Ltd., New York.
3. Organic Chemistry, VI edition, Robert T. Morrison, Robert N. Boyd.
4. Organic Chemistry, Vol-I by I. L. Finar.
5. Vogel' text book of practical organic chemistry, V edition, B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatehell.
6. Laboratory manual of Organic Chemistry by B. B. Dey and M. V. Sitaraman.
7. Practical Organic Chemistry by Mann F. G. and Saunders.
8. Fundamentals of analytical chemistry, 8th Edition, D. A. Skoog, D. M. West, Holler and Crouch.
9. Principles and Practice of Analytical Chemistry, F.W. Fifield and Kealey, 3rd edition, 2000, Blackwell Sci., Ltd. Malden, USA.
10. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.

THIRD SEMESTER

CHI HCT: 3.1. ADVANCED INORGANIC CHEMISTRY

Objectives:

- To understand the fundamental concepts of organometallic chemistry and general principles of homogeneous and heterogeneous catalysis.
- To learn the concepts of metal clusters, silicates and silicones.

Course outcome:

- Fundamental concepts of organometallic chemistry and synthesis, structure and bonding in different organometallics and their applications.
- Homogeneous and heterogeneous catalysts and their applications in the synthesis of organic compounds in industries.
- Chemistry of main group elements, metal clusters, silicates and silicones and their applications in day to day life.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animations are used in class room teaching.

Course content

UNIT-I

[16 HOURS]

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.

Ferrocene: Preparation, structure and bonding**. Metal-carbene and metal-carbyne complexes**.

Complexes containing alkene, alkyne, arene and allyl ligands: Preparation, structure and bonding.

UNIT-II

[16 HOURS]

General principles of Catalysis: Language of catalysis. Homogeneous and heterogeneous catalysts.

Homogeneous catalysis - Industrial Applications: Alkene hydrogenation and hydroformylation, The Wacker's process, Monsanto acetic acid process and L-DOPA synthesis, alkene oligomerizations, water-gas shift reactions. The Reppe reaction.

Heterogeneous catalysis –The nature of heterogeneous catalysts. Alkene polymerization: Ziegler-Natta catalysis, Fischer-Tropsch carbon chain growth. New directions in heterogeneous catalysis.

Zeolites as catalysts for organic transformation: Uses of ZSM – 5.

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

Biological and Medicinal Applications: Organomercury, organoboron, organosilicon and organoarsenic compounds.

UNIT-III

[16 HOURS]

Chemistry of main group elements: Diborane and its reactions, polyhedral boranes(preparation, properties, structure and bonding). Wade's rules, carboranes andmetallocarboranes. Borazines. Phosphazenes, S-N compounds.

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

Low and high nuclearity carbonyl clusters. Electron counting schemes in carbonyl clusters. The isolobal analogy.

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

Silicones: General methods of preparation, properties. Silicone polymers - silicone fluids, silicone greases, silicone resins, silicone rubbers and their applications.

References

1. Organometallic Chemistry, 2nd edition, R.C. Mehrothra and A. Singh, New Age International Publications (2006).
2. Fundamental Transition Metal Organometallic Chemistry - Charles M. Lukehart, Brooks, Cole Publishing Company (1985).
3. The Organometallic Chemistry of the Transition Metals, 4th edition, Robert H. Crabtree, Wiley Interscience, (2005).
4. Organometallics - A Concise Introdution, 2nd edition, ChistophElschenbroich and Albert Salzer VCH, (1992).
5. Inorganic Chemistry, 2nd edition, C.E. Housecroft and A.G. Sharpe, Pearson Education Ltd., (2005).
6. Inorganic Chemistry- 3rd edition, G.L. Miessler and D.A. Tarr, Pearson Education,(2004).
7. Basic Organometallic Chemistry - B.D. Gupta and A.J. Elias, Universities Press (2010).
8. Inorganic Chemistry Principles of Structure and Reactivity: James E. Huheey, Ellen A.
9. Keiter, Richard L. Keiter, Okhil K. Medhi, Delhi University, New Delhi (2006)
10. Chemistry of the Elements – N.N. Greenwood and A. Earnshaw, Pergamon Press (1985).
11. Inorganic Chemistry, 6th edition. D.F. Shriver, M. Weller. T. Overton, J. Rourke and F. Armastrong, Oxford University Press (2014).
12. Organometallic Chemistry and Catalysis, Didier Astruc, Springer (2007).
13. Transition Metal Organometallic Chemistry, Francois Mathey, Springer (2013).

CHO HCT: 3.2. ORGANOMETALLIC AND PHOTOCHEMISTRY

Objectives:

- To understand the fundamental concepts of photochemistry and pericyclic reactions.
- To learn the synthesis and reactions of organometallic compounds.
- To learn the asymmetric synthesis of organic compounds.

Course outcome:

- Basic concepts of photochemistry and pericyclic reactions and their usefulness in the synthesis of many organic compounds.
- Synthesis of organic compounds using different organometallic compounds as catalysts.

- Asymmetric synthesis of organic compounds using chiral compounds.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation is used in class room teaching.

Course content

UNIT-I

[16 HOURS]

Photochemistry: Light absorption and electronic transitions, Jablonski diagram, intersystem crossing, energy transfer, sensitizers, quenchers. Photochemistry of olefins, conjugated dienes, aromatic compounds, ketones- Norrish type-I and Norrish type-II reactions, enones, Paterno-Buchi reaction, di-pi- rearrangements, photooxidations, photoreductions.

Pericyclic reactions: Electrocyclic reactions: Stereochemistry, symmetry and Woodward-Hofmann rules for electrocyclic reactions, FMO theory of electrocyclic reactions, correlation diagram for butadiene to cyclobutene and hexatriene to cyclohexadiene systems. Cycloaddition reactions: Classification, analysis by FMO and correlation diagram method. Cycloaddition reactions: [2+2] and [4+2] cycloadditions- FMO and correlation diagram method Deils-Alder reaction, hetero Diels-Alder reaction and their applications. Intra and intermolecular 1,3-dipolar cycloadditions: involving nitrile oxide, nitrile imine, nitrile ylide and their application in organic synthesis. Sigmatropic reactions: Classification, stereochemistry and mechanisms. suprafacial and antarafacial shifts of H and carbon moieties. [3,3] and [5,5]- sigmatropic rearrangement, Claisen, Cope and aza-Cope rearrangement.

UNIT-II

[16 HOURS]

Chemistry of organometallic compounds: Synthesis and reactions of organolithium (n-BuLi, PhLi), organocadmium, organomagnesium (Grignard reagent), organoselenium and organotellurium. Organoaluminium reagents: Preparation, site selective and stereoselctive 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. Organocopper reagents: Gilmann reagent, preparation, reactions with aldehydes, ketones and imines. Application in the synthesis of brevicomin, 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. Organotin reagents: tributyltin hydride, Barton decarboxylation reaction, Barton deoxygenation reaction, Stille coupling, Stille-Kelley coupling reactions, Barton McCombie reaction, Keck stereoselective allylation and other applications.

UNIT-III

[16 HOURS]

Asymmetric synthesis: Definition, importance, mechanism, energy consideration, advantages and limitations, methods of determination of enantiomeric excess. Methods of asymmetric induction:

Topocity-Prochirality: Substrate selectivity - Diastereoselectivity and enantio-selectivity-Substrate controlled methods-use of chiral substrates - examples

Auxiliary controlled methods: Use of chiral auxiliaries - Chiral enolates-alkylation of chiral imines - Asymmetric Diels - Alder reaction

Reagent controlled methods: Use of chiral reagents - Asymmetric oxidation –Sharpless epoxidation - Asymmetric reduction - Use of lithium aluminium hydride and borate reagents. Synthesis and applications of oxazaborolidines, IPC-BBN, IPC2BH, (*S*)-BINAP-DIAMINE and (*R*)-BINAL-H. Use of (*R*,*R*)-DIPAMP, (*S*,*S*)-CHIRAPHOS, (*R*,*R*)-DIOP, SAMP, RAMP, *S*-Proline, *S*-PBMgCl, (-)-BOAlCl2, (+) and (-)-DET.

References

1. Organic Chemistry, VI edition, Robert T. Morrison, Robert N. Boyd.
2. Advance Organic Chemistry, IV edition, Jerry March.
3. Advance Organic Chemistry, III edition, Part-A and Part-B, Francis A. Carey and Rechard J. Sundberg.
4. Organic Chemistry, III edition, V. K. Ahluwalia and Rakesh Kumar Parashar.
5. Schaum's outline of theory and problems of Organic Chemistry, Harbert Meislich, Howard Nechamkin and Jocob Sharefkin.
6. Asymmetric synthesis, Garry Procter.
7. Mechanism in Organic Chemistry, VI edition, Peter Sykes.
8. Molecular reactions and photochemistry, Charles H. Depuy, Orville L. Chopman.
9. Modern methods of Organic synthesis, III edition, W. Carruthers.
10. Organometallics in Organic synthesis, J. M. Swan and D. Stc Black.
11. Organic chemistry by Clayden, Greeves, Warren and Wothers.

CHP HCT: 3.3. ADVANCED PHYSICAL CHEMISTRY

Objectives:

- To understand the concepts of enzyme kinetics, industrial catalysis and linear free energy relationship.
- To learn the electrochemical aspects of batteries and electroplating.
- To understand the mechanism of corrosion prevention of metals by different methods.
- To understand the fundamentals of X-ray crystallography.

Course outcome:

- Applications of reaction kinetics help in correlating the rates of biological and chemical reactions.
- Theory and applications of electrochemical systems helps in the field of e-waste management and protection of metals.
- Fundamentals of X-ray crystallography and structural interpretation by various X-ray diffraction techniques.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animation are used in class room teaching.
- Students will be assigned to solve the numerical problems to understand the concepts.

Course content

UNIT-I

[16 HOURS]

Homogeneous Catalysis: Electronic and structural effects on acidity and basicity. Hard and soft acids and bases. Acidity functions: Hammet acidity function, Zucker-Hammet hypothesis, Bonnett hypothesis. Industrial catalysis: Catalyst carrier, promoter, inhibitor and catalyst poison.

Enzyme kinetics: Effect of substrate concentration (Michaelis - Menton equation), Effect of pH, effect of catalysts and inhibitors (substrate, zeolite, Cr^{3+}, Fe^{2+} ZnO, U.V light), effect of temperature. A brief kinetic and mechanistic applications of glucose oxidase in the oxidation of glucose.

Linear Free Energy Relationship: Hammett equation, Taft equation, Okemoto Brown equation and its application to oxidation of amino acids and aromatic amines. Swain-Scott and Edward equation. Winstein - Grunwald relationship. Isokinetic relationship and significance of isokinetic temperature, Exner criterion.

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

UNIT-II

[16 HOURS]

Electrochemical cells and batteries: Introduction, galvanic and electrolytic cells, schematic representation of cells. Faradays's law, mass transfer in cells. Batteries: Classification, characteristics, primary, secondary and lithium batteries, fuel cells.

Electroplating: Definition, theory and mechanism of electroplating, effect of plating variables on the properties of electro deposits, comparative account of complexing and non-complexing baths (general treatment), additives on plating baths and their significance.

Metallic coating: Preparation of substrate surface, electroplating of Cu and Cr. Application of Au and Ag plating.

Corrosion: Types of corrosion, basis of electrochemical corrosion, theories and mechanism of wet corrosion. Thermodynamic aspects of corrosion. Current – potential relations (Evan diagram) in corrosion cells. Factors influencing the rate of corrosion: Metal and environmental factors. Kinetic aspects corrosion: Corrosion rate measurement by different methods – chemical and electrochemical methods. General aspects of corrosion prevention and control – designing aspects, effect of allying and surface modification. Corrosion prevention by painting, phosphating and anodic (passivation) and cathodic protection. Corrosion inhibitors: Introduction, classification, Characteristics and requirements of efficient corrosion inhibitors, Green inhibitors and their significance, Corrosion inhibition mechanism.

UNIT-III

[16 HOURS]

Fundamentals of 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.

Imperfections in atomic packing: 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, non-stoichiometry.

Imperfections and physical properties: electrical, optical, magnetic, thermal and mechanical properties.

References

1. Chemical Kinetics by K.J. Laidler, Tata McGraw-Hill Pub, Co Ltd, New Delhi.
2. Fundamentals of Chemical Kinetics, M. R. Wright, Harwood publishing, Chichesrer, 1999.
3. Kinetics and Mechanism of Chemical Transformation by J. Rajaram and J.C. Kuriacose, Macmillan, New Delhi.
4. Electrochemistry –Principles and Applications by E.G. Potter, Cleaver-Hume press Ltd, London.
5. Chemical and Electrochemical energy systems, R. Narayan and B. Viswanathan (University Press), 1998.
6. Industrial Electrochemistry, D. Pletcher and F. C. Walsh, Chapman and Hall, 2nd Edn, 1984.
7. An Introduction to Metallic Corrosion and its Prevention, Raj Narayan (Oxford – IBH, New Delhi), 1983.
8. Fundamentals of metallic corrosion, Philips A. Schweitzer, CRC press Taylor and Francis group, New York.
9. Corrosion prevention and control, Baldev Raj, U Kamachi Mudali & S. Rangarajan, Narora Publishing House, India.
10. Solid State Chemistry and its applications – A.R. West, John Wiley & Sons.
11. New Directions in Solid State Chemistry – CNR Rao and J. Gopalakrishna, Cambridge University Press.
12. Solid state chemistry, N. B. Hannay, PHI, New Delhi.
13. Principles of the Solid State – H.V. Keer, Wiley Eastern.

CHG HCT: 3.4. CHEMICAL SPECTROSCOPY

Objectives:

- To understand the basic concepts of spectroscopic techniques such as NMR, ESR, NQR, Mossbauer and photoelectron spectroscopy.
- To familiarize with the IR and mass spectroscopy.

Course outcome:

- Understand the spectroscopic techniques such as NMR, IR, UV, and MS for recording and interpretation of spectra.
- Understand the characterization of chemical compounds.
- Learnt electric and magnetic properties of radiation, molecules and bulk matter and solve the problems related to these properties.
- Understanding various fragmentation reactions of organic molecules.
- Predict the NMR, IR, UV, and MS spectra from a given molecular structure, including fragment-ions in MS.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animation are used in class room teaching.
- Students will be assigned to solve the spectroscopic problems to understand the interpretation of spectra.

Course content

UNIT-I

[16 HOURS]

NMR Spectroscopy: Magnetic properties of nuclei (magnetic moment, g factor, nuclear spin), effect of external magnetic field on spinning nuclei, Larmor precession frequency, resonance conditions, population of nuclear magnetic energy levels, relaxation processes, relaxation time, line width and other factors affecting line width. Chemical Shift: Standards employed in NMR, factors influencing chemical shift: electronegativity, shielding and deshielding, van der Walls deshielding magnetic anisotropy, H-bonding, diamagnetic and paramagnetic anisotropies, spin-spin coupling, chemical shift values and correlation for protons bonded to carbon and other nuclei, Instrumentation. Chemical shift equivalence and magnetic equivalence, effects of chiral centre, Karplus curve-variation of coupling constants with dihedral angle. Complex NMR Spectra: Simplification of complex spectra-isotopic substitution, increased magnetic field strength, double resonance and lanthanide shift reagents, Nuclear Overhauser Effect (NOE), FT-NMR, Spectroscopy and advantages. ^{13}C-NMR Spectroscopy, multiplicity-Proton decoupling-Noise decoupling-Off resonance decoupling-Selective proton decoupling - Chemical shift, application of ^{13}C, ^{19}F, ^{31}P, ^{11}B and ^{15}N. Applications of NMR: Structural diagnosis, conformational analysis, keto-enol tautomerism, H bonding. Solid state NMR and its applications.

Multiple resonance spectroscopy: Introduction to 2D-techniques: DEPT, COSY and NOESY.

UNIT-II

[16 HOURS]

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.

NQR Spectroscopy: Introduction, Principles, 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, magnetic splitting, measurement techniques and spectrum display, application to the study of $Fe^{2+}$and Fe^{3+}compounds; iron in very high oxidation states-Fe(V) and Fe(VI) nitride complexes; $Sn^{2+}$and Sn^{4+}compounds, nature of M-L bond, coordination number and structure, detection of oxidation states and an inter halogen compound $I_2Br_2Cl_4$.

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

UNIT-III

[16 HOURS]

IR spectroscopy: Introduction, instrumentation, sample handling, Characteristic group frequencies and skeletal frequencies. Finger print region, Correlation chart. Identification of functional groups- alkanes, alkenes, alkynes, aromatics, carbonyl compounds (aldehydes, ketones, esters and lactones), halogen compounds, sulphur and phosphours compounds, amides, lactums, 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.

Mass Spectrometry: Basic principles, Instrumentation -Mass spectrometer, interpretation of mass spectra, resolution, exact masses of nuclides, molecular ions, meta-stable ions and isotope ions. Different methods of ionization (chemical ionization, electron impact, field ionization, MALDI etc.). Fragmentation processes-representation of fragmentation, basic fragmentation types and rules. Factors influencing fragmentations and reaction pathways. McLafferty rearrangement. Fragmentations (fragmentation of organic compounds with respect to their structure determination) associated with functional groups- alkanes, alkenes, cycloalkanes, aromatic hydrocarbons, halides, alcohols, phenols, ethers, acetals, ketals, aldehydes, ketones, quinines, carboxylic acids, esters, amides, acid chlorides, nitro compounds, amines & nitrogen heterocycles. Fragmentation patterns of glucose, myrcene, nicotine, retro Diels-Alder fragmentation. Application in structure elucidiation and evaluation of heats of sublimation & ionization potential. Nitrogen rule. LC-MS and GC-MS, High resolution mass spectroscopy. Composite problems involving the applications of UV, IR, ^{1}H and ^{13}C-NMR and mass spectroscopic techniques. Structural elucidation of organic and inorganic compounds.

References

1. Organic Spectroscopy-3rd Ed.-W. Kemp (Pagrave Publishers, New York), 1991.
2. Spectrometric Identification of Organic Compounds - Silverstein, Bassler & Monnill (Wiley) 1981.
3. Spectroscopy of Organic Compounds-3rd Ed.-P.S. Kalsi (New Age, New Delhi) 2000.
4. E.A.V. Ebsworth, D.W.H. Ranklin and S. Cradock: Structural Methods in Inorganic Chemistry, Blackwell Scientific, 1991.
5. J. A. Iggo: NMR Spectroscopy in Inorganic Chemistry, Oxford University Press, 1999.
6. C. N. R. Rao and J. R. Ferraro: Spectroscopy in Inorganic Chemistry, Vol I & II (Academic) 1970.
7. Spectroscopy, B. P. Straughan and S. Salker, John Wiley and Sons Inc., New Yourk, Vol.2, 1976.
8. Application of Absorption Spectroscopy of Organic Compounds, John R. Dyer, Prentice/Hall of India Private Limited, New Delhi, 1974.
9. Organic Spectroscopy, V. R. Dani, Tata McGraw-Hall Publishing Company Limited, New Delhi. 1995.
10. Interpretation of Carbon-13 NMR Spectra, F.W. Wehrli and T. Wirthin, Heyden, London, 1976.
11. NMR spectroscopy-Powai

CHA SCP: 3.1/4.1. ANALYTICAL CHEMISTRY PRACTICALS-II

[64 HOURS]

Objectives:

- To familiarize with the handling of instruments in the quantitative analysis of various samples.
- To understand the analysis of waste water, soil samples and biological samples.

Course outcome:

- Different chemistry such as redox, acid-base and complexometric titrations by performing various experiments in the determination of pharmaceutical, industrial and food samples.
- Analysis of soil and water samples of environmental interest.
- Analysis of biological fluids using spectrophotometric, chromatographic and titrimetric methods.

Pedagogy:

- Each student performs experiments as per the protocol in practical classes.
- Computer aided applications are used for the evaluation of experimental results.

Course experiments

PART-A

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 indophenols.
3. Determination of aluminium and magnesium in antacids by EDTA titration.
4. Analysis of a copper-nickel alloy sample for copper and nickel by EDTA titration using masking and selective demasking reactions.
5. Determination of saccharin in tablets by precipitation titration.
6. Determination of ascorbic acid in goose berry/bitter gourd by titrimetry and spectrophotometry using *N*-bromosuccinimide (NBS).
7. Analysis of a mixture of iron(II) and iron(III) by EDTA titration using *p*H control.
8. Potentiometric titration of a mixture of chloride and iodide.
9. Determination of sulpha drugs by potentiometry using $NaNO_2$ and iodometric assay of penicillin.
10. Polarographic determination of copper and zinc in brass.
11. Determination of manganese in steel by extraction-free spectrophotometry and molybdenum in steel by extractive spectrophotometry.
12. Determination of iron in mustard seeds and phosphorous in peas by spectrophotometry.

PART-B

1. Analysis of waste waters for DO and COD by titrimetry.
2. Analysis of a ground water sample for sulphate by titrimetry (EDTA) and turbidimetry.
3. Potentiometric determination of formula and stability constant of a silver-ammonia complex ion.
4. Photometric and potentiometric titration of iron(III)/copper with EDTA.
5. Analysis of brackish water for chloride content by a**)** spectrophotometry (mercuric thiocyanate method), b) conductometry (silver nitrate) and c**)** potentiometry (silver nitrate).
6. Ascorbic acid determination in natural orange juice by coulometry.
7. Analysis of waste water for:
   a) Phosphate by molybdenum blue method
   b) Ammonia-nitrogen by Nessler’s method
   c) Nitrite-nitrogen by NEDA method
8. Analysis of a soil sample for:
   a) Calcium carbonate and organic carbon by titrimetry.
9. Analysis of a soil sample for:
   a) Available phosphorus by spectrophotometry.
   b) Nitrate-nitrogen/nitrite nitrogen/ammonia nitrogen by spectrophotometry.
10. Analysis of urine for:
    a) Urea and uric acid by titrimetry snd spectrophotometry.
    b) Sulphate by precipitation titration after ion-exchange separation.
    c) Sugar by Benedict’s reagent.
11. Analysis of blood for:

a) Cholesterol by spectrophotometry
b) Bicarbonate by acid-base titration.

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.
5. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003 Pearson Education Pvt. Ltd., New Delhi.
6. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
7. Pharmaceutical Drug Analysis by Ashutoshkar, New Age International Publishers, New Delhi, 2005.
8. Practical Pharmaceutical Chemistry, Ed. A. H. Geckett, J. B. Stenlake, 4th edition. Part I and II, CBS Publishers, New Delhi.
9. Quantitative Analysis of Drugs in Pharmaceutical Formulations, P. D. Sethi, 3rd edition, CBS Publishers & Distributors, New Delhi, 1997.
10. Practical Clinical biochemistry methods and interpretations, R. Chawla, J.P. Bothers Medical Publishers (P) Ltd., 1995.
11. Laboratory Manual in Biochemistry, J. Jayaraman, New Age International Publishers, New Delhi, 1981.
12. Practical Clinical Biochemistry, Harold Varley and Arnold.Hein mann, 4th edition.
13. Environmental Science: Laboratory Manual, Maurice A. Strabbe, The C.V. Mosbey Co. Saint Loucs, 1972.
14. Experiments on Water Pollution, D.I. Williams and D. Anglesia, Wayland Publishers Ltd., England, 1978.
15. Experiments on Land Pollution, D.I. Williams and D. Anglesia, Wayland Publishers Ltd., England, 1978.
16. Experiments in Environmental Chemistry, P.D. Vowler and D.W. Counel, Pergamon Press, Oxford 1980.
17. Manual Soil Laboratory Testing, vol. I, K.H. Head, Pentech Press, London 1980.

CHI SCP: 3.2/4.2. INORGANIC CHEMISTRY PRACTICALS-II

[64 HOURS]

Objectives:

- To familiarize with the instrumental methods of analysis for determining metals present in the different samples.
- To familiarize with the preparation and characterization of different inorganic complexes.

Course outcome:

- Determination of alloy samples and understanding the electrochemical deposition of metals.
- Preparation and characterization of coordination compounds.
- Determination of composition, stability constant and magnetic susceptibility of metal complexes.

Pedagogy:

- Each student performs experiments as per the protocol in practical classes.
- Spectroscopic tools are applied for the characterization of the synthesized complexes.

Course experiments

PART-A

1. Determination of bismuth, cadmium and lead in a mixture: Analysis of a low melting alloy (Wood's alloy).
2. Simultaneous spectrophotometric determination of chromium and manganese in a steel solution.
3. Determination of chromium(III) and iron(III) in a mixture: Kinetic masking method.
4. Electrogravimetric determination of:
   a) Copper in copper sulphate
   b) Nickel in nickel suphate
   c) Copper and nickel in alloy solution
   d) Lead in lead nitrate.
5. Flame photometric determination of the following metal ions from different samples:
   a) sodium b) potassium and c) sodium and potassium in a mixture.
6. Polarographic estimation of cadmium and zinc.
7. Determination of iron as the 8-hydroxyquinolate by solvent extraction method.
8. Quantitative determination of nickel using dithizone and 1,10-phenanthroline by synergistic extraction.
9. Spectrophotometric determination of the *p*Ka value of methyl red.
10. Semimicro gravimetric determination of aluminium,

PART-B

11. Preparation and characterization of:
    a) Chloropentammine cobalt(III) chloride
    b) Estimation of chloride in a complex by potentiometric or ion-exchange method
    c) Record the electronic absorption spectrum of a complex and verify TanabeSugano diagram.
12. Preparation of *cis*- and *trans*- dichlorobis(ethylenediammine) cobalt(III)chloride. Record the UV-Vis spectra and compare it with *cis*-form. Measure the molar conductance.
13. Preparation of hexammine cobalt(III) chloride and estimate cobalt ion.
14. Determination of magnetic susceptibility of any two compounds/complexes by Gouy method.
15. Determination of the composition of iron-phenanthroline complex by:
    (a) Job's method
    (b) mole-ratio method and
    (c) Slope-ratio method.
16. Determine the stability constant of iron-tiron/iron-phenanthroline by Turner-Anderson method.
17. Preparation of potassium tris(oxalato)ferrate(III) and estimate the metal ion.
18. Preparation of acetyl acetonatomanganese(III) complex.
19. Preparation of tris(en)nickel(II) chloride and hexamine nickel(II) chloride complexes. Record electronic spectra and evaluate spectrochemical series.
20. Using chloropentammine cobalt(III) chloride, prepare nitro and nitritopentammine cobalt(III) chloride. Record the IR spectra of the isomers and interpret.

21. Estimate the chloride ion in a given complex by silver nitrate titration after ion-exchange separation.

22. **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, 5^{th} 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) 7^{th} edition.
8. Spectrophotometric Determination of Elements – Z. Marczenko

CHO SCP: 3.3/4.3. ORGANIC CHEMISTRY PRACTICALS-II

[64 HOURS]

Objectives:

- To understand the concepts of isolation and purification of natural products.
- To familiarize with the estimation of different functional groups in organic compounds.

Course outcome:

- The isolation of caffeine, carotene, lycopene, cincole, azelaic acid and piperine from respective natural sources.
- Estimation of ketones, sugars, nitro and amino groups in natural products.
- Interpret UV, IR, NMR and MS data of different organic compounds.

Pedagogy:

- Each student performs experiments as per the protocol in practical classes.
- Spectroscopic tools are applied for the characterization of isolated natural products.

Course experiments

PART-A

1. Fractional crystallization: separation of mixture of naphthalene and biphenyl.
2. Thin layer chromatography: Separation of plant pigments.
3. Isolation of piperine from pepper.
4. Isolation of caffeine from tea.
5. Isolation of azelaic acid from castor oil.
6. Isolation of carotene from carrot.
7. Isolation of lycopene from tomato.
8. Isolation of cincole from eucalyptus leaves.

PART-B

Isolation of natural products & estimations:

1. Estimation of ketones by haloform reaction.
2. Estimation of sugars by Bertrand's method.
3. Estimation of nitro groups.
4. Estimation of amino group.
5. Determination of iodine value of an oil or fat.
6. Determination of saponification value of oil.
7. Determination of equivalent weight of carboxylic acid by silver salt method

Interpretation of Spectra: Structural elucidation of some simple organic compounds by UV, IR, NMR and mass. Spectra have to be provided by the Examiners.

References

1. Vogel' text book of practical organic chemistry, V edition, B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatehell.
2. Elementary practical organic chemistry, Part-III: Quantitative organic analysis, By Arthur I, Vogel.
3. Laboratory manual of Organic Chemistry by B. B. Dey and M. V. Sitaraman.
4. Practical Organic Chemistry by Mann F. G. and Saunders.
5. Natural products: A laboratory guide by Raphael Ikhan.

CHP SCP: 3.4/4.4. PHYSICAL CHEMISTRY PRACTICALS-II

[64 HOURS]

Objectives:

- To understand the significance of various factors influencing the reaction rate in proposing the reaction mechanism.
- To understand electrochemical and spectrophotometric methods of quantification of samples, and also determination of physico-chemical parameters of some important samples.

Course outcome:

- Students can able to develop experimental skill and interpretation of plausible mechanisms of reactions.
- Gain practical knowledge on the theoretical basis of electrochemistry, thermodynamics, and spectrophotometry experiments.
- This helps in academics, research and industries.

Pedagogy:

- Each student performs experiments as per the protocol in practical classes.
- Electrochemical and spectrophotometric tools are used to conduct the experiments.

Course experiments

PART-A

1. Determination of order of reaction for the acid hydrolysis of methyl acetate and evaluation of activation parameters.
2. Evaluation of Arrhenius parameters for the reaction between $K_2S_2O_8$ and KI (First order reaction).

3. Study of kinetics of autocatalytic reaction between oxalic acid and $KMnO_4$ and determine the order of reaction with respect to $KMnO_4$.
4. Kinetics of saponification of ethyl acetate by conductivity method and study the effect of dielectric constant of the medium (using CH_3OH).
5. Study of effect of salt (ionic strength) on the kinetics of reaction between potassium persulphate and potassium iodide (second order reaction).
6. Spectrophotometric kinetics of oxidation of indigocarmine (IC) by chloramine-T (CAT) – Determination of order of reaction with respect to [CAT] and [IC].
7. To study the acid catalysed kinetics of oxidation of glycine by chloramine-T (CAT) - determination of order of reaction with respect to [CAT] and [glycine].
8. Study the phase diagram of three component system (Glacial acetic acid-Chloroform-water system / Glacial acetic acid-Acetone-Water system).
9. Study the rate of corrosion and inhibition efficiency of an inhibitor (thiourea) on mild steel/Al/Cu by weight loss method.

PART-B

1. Conductometric titration of orthophosphoric acid against NaOH.
2. Conductometric titration of a mixture of HCl, CH_3COOH and $CuSO_4$ against NaOH.
3. Conductometric titration of thorium nitrate with potassium tartarate.
4. Potentiometric titration of mixture of weak acids (Acetic acid and Monochloacetic acid) against NaOH.
5. Dwtermination of pK_a values of phosphoric acid by potentiometric / pH metric method.
6. Potentiometric titration of mixture of KCl+KBr+KI against $AgNO_3$.
7. Potentiometric titration of FAS against Ceric sulphate and sodium metavenadate, determine the concentration of FAS and redox potential.
8. Potentiometric titration of lead nitrate against EDTA and determine the concentration of lead nitrate solution.
9. Determination of *p*K value of an indicator (methyl orange/methyl red).
10. Spectrophotometric analysis of a mixture of (a) $KMnO_4$ and $K_2Cr_2O_7$.
11. Study of complex formation between ferric salt and salicylic acid.

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.

SOFT CORE PAPERS

CHA SCT: 3.1. ELECTROCHEMICAL METHODS OF CHEMICAL ANALYSIS

Objectives:

- To understand the rate of chemical reactions by carrying out kinetic experiments.
- To understand basic principles, instrumentation and applications of electrochemistry.

Course outcome:

- Basic concepts of electrochemical methods and applications of potentiometry and coulometric methods.
- Theory, instrumentation and applications of electrogravimetric, voltammetric and stripping methods.
- Chemical sensors and biosensors.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and information and communications technology are used in class room teaching.
- Students will be assigned to solve the numerical problems to understand electrochemical concepts.

Course content

UNIT-I

[16 HOURS]

Introduction to electrochemical methods and types: Definitions-electrochemical, galvanic and electrolytic cells, half-cell reactions, anode and cathode, reversible cell, standard hydrogen electrode (SHE), electrode potential (E), standard electrode potential (E^0), theoretical cell potential, liquid junction potential, ohmic drop, IR, overvoltage, concentration over potential.
Activity-dependence of electrode potentials- the Nernst equation, reference electrode-calomel and Ag-AgCl electrodes.

Potentiometry: Electrode systems, metallic indicator electrodes. Membrane electrodes, Ion-selective electrodes-electrode response and selectivity of glass electrode for pH measurement, errors in the use of glass electrode. Glass electrodes for the measurement of cations other than hydrogen -Solid state electrodes, liquid membrane electrodes. Ion-selective field effect transistors (ISFETS). Gas sensing electrodes. Direct potentiometry: Chemical and environmental applications. Potentiometric biosensors. Potentiometric titrations- acid-base, precipitation and redox titrations. Null-point potentiometry.

Coulometric methods of analysis: Basis, Faraday's law and current efficiency. Characterizing coulometric methods. Controlled-potential coulometry- selecting a constant potential, minimising electrolysis time. Instrumentation and applications. Characterisation applications: determining the number of electrons involved (n) in a reaction. Controlled-current coulometry-minimising current efficiency, detecting the end point.

Instrumentation: current sources and cells. Comparing conductometric and conventional titrations. Applications. Automated coulometric titrations.

UNIT-II

[16 HOURS]

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

Voltammetry and polarography: Introduction. Electrodes. Polarographic principles- polarographic current, polarographic potential, polarographic maxima, oxygen removal. Qualitative and quantitative analyses. AC polarography. Pulse polarography. Differential pulse polarography and square wave polarography. Trace analysis by pulse polarography. Inorganic, organic, clinical and environmental applications. Characterisation applications- electrochemical reversibility and determination of ‘n'. Determination of equilibrium constants for coupled chemical reactions. Voltammetric principles- Voltammetry at solid electrodes- hydrodynamic voltammetry, triangular voltammetry or cyclic voltammetry. Modified electrodes. Amperometry, amperometric titration. Biamperometry.
Stripping methods-anodic and cathodic stripping methods. Electrodeposition step and voltammetric deposition step. Applications of stripping methods. Voltammetry with micro electrodes.
Chemical sensors and biosensors: Sensors, electrochemical sensors, optical sensors, thermal and mass-sensitive sensors, sensor arrays.

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

CHI SCT: 3.2. FRONTIERS IN INORGANIC CHEMISTRY

Objectives:

- To understand the basic concepts, synthesis and applications of materials.
- To learn the properties, fabrication and characterization of nanomaterials.

Course outcome:

- Gain knowledge on design and synthesis of new inorganic materials.
- Fabrication and characterization of nanomaterials.
- Applications of ceramics, pigments, silicates and biomaterials.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animations are used in class room teaching.

Course content

UNIT-I

[16 HOURS]

Materials chemistry: Historical Perspectives. Design of new materials through a Critical Thinking Approach. Materials sustainability.
Synthesis of materials: The formation of bulk material by different methods.
Defects and ion transport: Extended defects. Atom andion diffusion.Solid electrolytes.
Metal oxides, nitrides and fluorides: Monoxides of the 3d metals, higher oxides and complex oxides, oxide glasses, nitrides and fluorides.
Sulfides, intercalation compounds and metal rich phases: Layered MS2 compounds and intercalation, Chevrel phases.
Ceramic materials: Sol-gel process and applications of biomaterials of ceramics.
Inorganic pigments: Coloured pigments, white and black inorganic materials.
Molecular materials and fullerides: Fullerides, 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.

UNIT-II

[16 HOURS]

Nanomaterials- an Introduction.
Fundamentals-Terminology and history.
Characterization and fabrication: Top-down and bottom-upfabrication. Solution based synthesis of nanoparticles. Vapour-phase synthesis of nanoparticles. Templated synthesis of nanomaterials using frameworks, supports and substrates. Sonochemical microwave methods for the synthesis of nanoparticles.
Structural study of nanocomposites by different methods.
Nanostructures and properties
One-dimensional control: carbon nanotubes and inorganic nanowires.
Two-dimensional control: grapheme, quantum wells and solid-state super lattices.
Three-dimensional control: mesoporous materials and composites.
Some applications of inorganic/organic/polymeric materials: Optical, electrical, magnetic, and chemical and biosensors.

References

1. Inorganic Chemistry, 4th edition. P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Oxford University Press (2006).
2. Inorganic Chemistry Principles of Structure and Reactivity: James E. Huheey, Ellen A. Keiter, Richard L. Keiter, Okhil K. Medhi, Delhi University, New Delhi (2006)**.**
3. Chemistry of the Elements – N.N. Greenwood and A. Earnshaw, Pergamon Press (1985).
4. Industrial Inorganic Chemistry – 2nd edition. K.H. Buchel, H.H. Moretto and P. Woditsh, Wiley - VCH (2000).
5. 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).
7. Inorganic Chemistry, 3rd edition. G.L. Miessler and D.A. Tarr, Pearson Education (2004).
8. Inorganic Chemistry, 2nd edition. C.E. Housecroft and A.G. Sharpe, Pearson Education.

CHO SCT: 3.3. CHEMISTRY OF NATURAL PRODUCTS-II

Objectives:

- To familiarize with the chemical concepts of alkaloids and steroids.
- To learn the structural elucidation and biological importance of alkaloids and steroids.

Course outcome:

- Chemistry of alkaloids and their biological significances.
- Synthesis and characterization of several alkaloids and steroids.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animations are used in class room teaching.

Course content

UNIT-I

[16 HOURS]

Alkaloids: Introduction, classification, isolation and general methods of structural elucidation of alkaloids. Classification of alkaloids. Biological importance of alkaloids. Structural elucidation of nicotin, papavarine, quinine, reserpine and morphine. Biosynthesis of alkaloids (nicotin, conine and cocaine).

UNIT-II

[16 HOURS]

Steroids: Introduction, Structural elucidation of cholesterol, bile acids, Ergosterol and its irradiation products. Sex hormones and corticosteroids: Synthesis of estrone, progesterone, androsterone, testosterone. Barton reaction for the synthesis of aldosterone. Brief discussion of homosteroids, norsteroids and oral contraceptives. Biological significance of anabolic steroids.

References

1. Organic Chemistry, VI edition, Robert T. Morrison, Robert N. Boyd.
2. Organic Chemistry, Vol-II by I. L. Finar.
3. Schaum's outline of theory and problems of Organic Chemistry, Harbert Meislich, Howard Nechamkin and Jocob Sharefkin.
4. Natural products: Their chemistry and biological significance, J. Mann, R. S. Davidson, J. B. Banthorpe and J. B. Harborne.

CHP SCT: 3.4. MATERIALS CHEMISTRY

Objectives:

- To familiarize with the preparation and characterization of different types of nanomaterials.
- To learn the properties and applications of semiconductors and superconductors.

Course outcome:

- Understand the fundamentals and importance of different types of nanomaterials, their methods of preparation and characterization by different techniques.
- Basic aspects of semiconductors and superconductors, their properties and applications.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animations are used in class room teaching.

Course content

UNIT-I

[16 HOURS]

Chemistry of Nanomaterials: Fundamentals and importance, metal nanoclusters, magic numbers, theoretical modelling of nanoparticles, geometric structure, electronic structure, reactivity, fluctuations, magnetic clusters, bulk to nano transitions. Semiconducting nanoparticles: optical properties, photo fragmentation, Coulombic explosion.

Carbon nanoparticles: Introduction, carbon molecules, nature of carbon bond, new carbon structure. Carbon clusters: Small carbon clusters, C_{60}: Discovery, structure, alkali doping, super conductivity. Fullerenes and other bulky balls. Carbon nano-tubes: Fabrication structure, electrical properties, vibrational properties, mechanical properties. Quantum dots, Graphene, and applications of nanomaterials.

Methods of preparation: Plasma arc, Chemical vapour deposition (CVD), sol-gel, silica-gel, hydrolysis, condensation, polymerization of monomers to form nanoparticles, solvothermal, and hydrothermal methods, electrochemical, ball milling and pulsed laser methods. Characterization of nanomaterials (X- ray, IR, UV and SEM).

UNIT-II

[16 HOURS]

Semiconductors: Metals, insulators and 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: Introduction, critical temperature and zero resistivity, Meissner effect, critical magnetic field and its variation with temperature. Type - I and II super conductors, specific heat, isotope effect, basic concepts of BCS theory. High temperature (Tc) superconductors and its applications.

References

1. Introduction to Nanotechnology, Charles P. Poole. Jr. and Frank J. Owens, Wiley-Interscience, Joh Wiley and Sons Inc, 2006.
2. Nanotechnology, Richard Booker and Earl Boysen, Wiley.
3. Nanometerials, A.K. Bandopadhyay, New Age International, 2nd edition.
4. Nanotechnology - Importance and Applications, M. H. Fulekar, Ink International publishing.
5. Solid State Chemistry – N.B. Hannay.
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).

FOURTH SEMESTER

CHI HCT: 4.1. BIOINORGANIC CHEMISTRY

Objectives:

- To understand the structural parameters of metallo-proteins and their biological role.
- To learn the biological properties of metal complexes in chemo and radio therapeutics.

Course outcome:

- Structural building blocks of proteins, nucleic acids and their metal ion interactions. Biological role of Na/K channel, Ca, Vit B12, and coenzymes.
- Biochemical reactions of several metallo-enzymes and oxygen transport proteins.
- Medicinal applications of metals and metal complexes, and also treatment of toxicity due to heavy metal ions.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animations are used in class room teaching.

Course content

UNIT-I

[16 HOURS]

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 O_2. Phosphorylation and respiratory chain. Oxidative phosphorylation.

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

Biochemistry of calcium: Introduction - comparison of Ca^{2+} and Mg^{2+}. 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. Photosystems.

UNIT-II

[16 HOURS]

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 O2--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, leucineaminopeptidase and carbonic anhydrase.

UNIT-III

[16 HOURS]

Medicinal Inorganic Chemistry: State of the Art, New Trends, and a Vision of the Future: 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, **Cancer Therapy**: Current Status and Mechanism of Action of Platinum-Based Anticancer Drugs. Non-platinum anticancer agents.

Gold-Based Therapeutic Agents: **A New Perspective**: Uses for the treatment of rheumatoid arthritis, **Diabetes**: Vanadium and diabetes,

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

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 - EiichiroOchiai, Academic Press, (2008).
7. Bioinorganic Chemistry: A Short Course - 2nd edition, R.M. Roat-Malone, Wiley Interscience, (2007).
8. Medicinal Applications of Coodination 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).
11. Essentials of Inorganic Chemistry, K. A. Strohfeldt, John Wiley and Sons Ltd.,(2015).
12. Bioinorganic Medicinal Chemistry (Ed) EnzoAlessio, Wiley-VCH Verlag and Co., (2011).

CHO HCT: 4.2. HETEROCYCLIC AND BIOORGANIC CHEMISTRY

Objectives:

- To familiarize with the chemistry of heterocyclic compounds.
- To learn the synthesis and biological importance of carbohydrates, proteins and nucleic acid.

Course outcome:

- Structure, reactivity and synthesis of several heterocyclic compounds.
- Synthesis, industrial and biological importance of carbohydrates.
- General synthesis of amino acids, peptides, nucleic acids and their biological significance.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animations are used in class room teaching.

Course content

UNIT-I

[16 HOURS]

Nomenclature of heterocyclic compounds. Structure, reactivity, synthesis and reactions of furan, pyrrole, thiophene, indole, pyridine, quinoline, isoquinoline, pyrazole, imidazole, pyrone, coumarin, chromones, pyrimidines, purines. Synthesis and synthetic applications of azirines & aziridines, azetidines, oxazolines, isoxazolines, isoxazole, triazole and azepines and benzodiazepines.

UNIT-II

[16 HOURS]

Carbohydrates: Carbohydrates: Introduction, Ring size determination of monosaccharides, configuration and conformations of monosaccharides, anomeric effect, Hudson's rules, epimerization and mutarotation. 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.

UNIT-III

[16 HOURS]

Amino Acids: General structure, physiological properties, protection of functional groups.

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 quartenary structure determination, denaturing and renaturing of proteins.

Nucleic acids: Introduction, structure and synthesis of nucleosides and nucleotides, protecting groups for hydroxy group in sugar, amino group in the base and phosphate functions. Methods of formation of internucleotide bonds: DCC, phosphodiester approach and phosphoramide methods. Solid phase synthesis of oligonucleotides. Structure of RNA and DNA, Crick-Watson model, role of nucleic acids in the biosynthesis of proteins.

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

References
1. Organic Chemistry, VI edition, Robert T. Morrison, Robert N. Boyd.
2. Organic Chemistry, Vol-II by I. L. Finar.
3. Schaum's outline of theory and problems of Organic Chemistry, Harbert Meislich, Howard Nechamkin and Jocob Sharefkin.
4. Natural products: Their chemistry and biological significance, J. Mann, R. S. Davidson, J. B. Banthorpe and J. B. Harborne.
5. A text book of synthetic drugs, O. D. Tyagi and M. Yadav.
6. Synthetic drugs, Gurdeep R. Chatwal.
7. Carbohydrate Chemistry and applications of carbohydrates, K. M. Lokanatha Rai.
8. Heterocyclic chemistry by Achison.
9. Heterocyclic chemistry by Smith and Joule.
10. Heterocyclic chemistry by Pacquete.

CHP HCT: 4.3. NUCLEAR, RADIATION AND PHOTOCHEMISTRY

Objectives:

- To understand the theory and applications of photochemistry.
- To learn the fundamentals and physico-chemical applications of radiation chemistry.
- To familiarize with the concepts of nuclear chemistry including radiochemical separation techniques and nuclear power reactors.

Course outcome:

- Understand the principles of photochemistry, its experimental techniques and applications.
- Fundamentals of radiation chemistry, experimental methods of detection of radiation and applications of radioisotopes.
- General aspects of nuclear chemistry, different types of nuclear reactions, production and separation of radioisotopes and also basic features of different types of nuclear reactors.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animations are used in class room teaching.

Course content

UNIT-I

[16 HOURS]

Nuclear chemistry: Nuclear stability – nuclear forces, packing fraction, binding energy, liquid drop, shell and collective models. Radioactive decay – General characteristics, decay kinetics, parent –daughter decay growth relationships, determination of half-lives. Brief survey of alpha, beta and gamma decays. Nuclear reactions – Bethe’s notation, types of nuclear reactions – specific nuclear reactions, photonuclear reactions, Oppenheimer – Phillips process, spallation reactions, Szilard-Chalmers process. Definition of Curie and related calculations. Production of radioisotopes and labelled compounds by bombardment.

Radiochemical separation techniques: carriers, solvent extraction and ion ion-exchange methods.

Nuclear power reactors: Types of nuclear power reactors, basic features and components of nuclear power reactors. An introduction to breeder reactors.

UNIT-II

[16 HOURS]

Radiation chemistry: Introduction, units, interaction of electromagnetic radiation with matter, G-value, LET of radiation. Chemical dosimetry - Fricke and ceric sulphate dosimeters. Radiolysis - cysteine, water and biphenyl. Radioisotopes as tracers, use of isotopic tracers in the elucidation of reaction mechanism, structure determination and solubility of sparingly soluble substances. ^{14}C dating, medical applications of isotopic tracers. Physico-chemical applications – isotope dilution method, activation analysis and radiometric titrations. Hazards in radiochemical work and radiation protection.

Radiation detection and measurement: Experimental techniques in the assay of radioisotopes. Radiation detectors – ionization chambers, proportional and Geiger-Muller counters – G.M. Plateau, dead time, coincidence loss, determination of dead time. Scintillation and semiconductor radiation detectors.

UNIT-III

[16 HOURS]

Photochemistry: Introduction to photochemistry, laws of photochemistry, laws of light absorption, quantum yield and its determination, factors affecting quantum yield, Actinometry - Uranyloxalate and potassium ferrioxalate actinometers, acetone and diethylketone actinometers. Term symbols for atoms and its significance. Photochemical properties of electronically excited molecules, nature of changes on electronic excitation, shapes of absorption band and Frank Condon principle. Experimental techniques to determine the intermediates in photochemical reactions. Photosensitization: by mercury, dissociation of H_2. Photochemical kinetics of: Decomposition of CH_3CHO, dissociation of HI and formation of HCl. Fluorescence and phosphorescence – theory and applications. Resonance fluorescence and quenching of fluorescence, Kinetics of colliosional quenching (Stern-Volmer equation).

Photocatalyst – Principle, application of ZnO/TiO_2 photocatalysts in the photo cleavage of dyes, environmentally hazardous waste and industrial effluents. Effect of photo degradation on COD value.

References

1. Photochemistry, Calvert and Pitts, Wiley, New York (1996).
2. Fundamentals of Photochemistry, Gohatgi-Mukherjee, New Age International Ltd., 1986.
3. Principles and Applications of Photochemistry, R. P. Wayne, Elsevier, New York (1970).
4. Photochemistry, Paul Suppan, RSC, London (1994).
5. Introduction to Semiconductor Materials and devices, M. S. Tyagi, John Wiley & Sons, 1991.
6. Nuclear Chemistry by Friedlander and Kennedy, John Wiley and Sons (1987).
7. Essentials of Nuclear Chemistry by H.J. Arnikar, Eastern Wiley (1990).
8. Nuclear Chemistry by U.N. Dash, Sultan Chand and Sons (1991).
9. Fundamentals of Radiochemistry by D.D. Sood, A.V.R. Reddy and N. Ramamoorthy**.**
10. Nuclear Radiation Detectors by S.S. Kapoor and Ramamoorthy, Wiley Eastern (1986).

CHA HCT 4.4. OPTICAL, THERMAL AND KINETIC METHODS OF ANALYSIS

Objectives:

- To understand the theory, instrumentation and applications of atomic emission spectroscopy.
- To learn the principles, instrumentation and applications of thermal methods of analysis.
- To familiarize with the concepts of kinetic methods of analysis.

Course outcome:

- Learnt the theory, instrumentation and applications of different types of atomic emission spectroscopy.
- To study the stages of thermal degradation patterns of materials using TGA and DTA techniques.
- To describe the general form of a (differential) rate law and describe how the rate of a chemical reaction depends on the concentrations of species that appear in the rate law.
- To describe the relationship between the order of a reactant and the stoichiometric coefficient for the reactant in the overall balanced chemical equation.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animations are used in class room teaching.
- Students will be assigned numerical problems to understand the concepts.

Course content

UNIT-I

[16 HOURS]

Atomic and molecular spectrometry-Electromagnetic radiation, atomic energy levels, molecular energy levels, transitions, quantitative spectrometry, Beer-Lambert's law.

Atomic spectrometry-Atomic structure and spectra, intensity of spectral lines.

Arc/spark atomic (optical) emission spectrometry- Principles, instrumentation, sample preparation, qualitative and quantitative analysis, applications

Glow discharge atomic emission spectrometry-principles, instrumentation, applications.

Plasma emission spectrometry- Principles, instrumentation, sample introduction, analytical measurements and applications.

Inductively coupled plasma-mass spectrometry (ICP-MS)-Principles, instrumentation and applications.

Flame emission spectrometry-principles, instrumentation, flame characteristics, flame processes, emission spectra. Quantitative measurements and interferences. Applications of flame photometry and flame atomic emission spectrometry.

Atomic absorption spectrometry- Principles, absorption of characteristic radiation. Instrumentation-sharp line sources- hallow cathode lamps, electrodeless discharge tubes. Sample vaporization- flame vaporization, flameless vaporization, vaporization by reduction and hydride generation. Quantitative measurements and interferences. Applications of AAS.

Atomic fluorescence spectrometry-Principles, instrumentation and applications.

X-ray emission spectrometry- Principles, instrumentation and applications.

Molecular fluorescence spectrometry- Theory- relaxation processes, excitation and fluorescence spectra, fluorescent species, factors affecting fluorescence, effect of concentration on intensity, fluorescence instruments, applications of fluorescence methods. Molecular phosphorescence- phosphorometry, chemiluminescence methods.

UNIT-II

[16 HOURS]

Thermal methods of analysis: Introduction, **Thermogravimetric analysis (TGA):** Introduction, 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.

Microcalorimetry: Micro-DSC instrumentation, Applications of Micro-DSC, Isothermal titration calorimetry, Microliter-flow calorimetry.

UNIT-III

[16 HOURS]

Kinetic methods of analysis: Analytical uses of reaction rates relative, basis of reaction rate methods, rate laws-first and second order reactions relative rates of reactions, analytical utility of first or pseudo first order reactions, determination of reaction rates, types of kinetic methods– differential methods, integral methods, multicomponent analysis-neglect of reaction of slow-reacting component, logarithmic extrapolation method, reaction rate method, applications-catalyzed reactions, measurement methods for catalyzed reactions, micro determination of inorganic species like iodide, selenium, cobalt & mercury in complex materials, determination of organic species, non-catalytic reactions. Applications of enzyme-catalysed reactions for the analysis of substratesstoichiometric and rate methods, determination of urea, uric acid, blood glucose, galactose and blood alcohol, determination of enzymes-LDH, GOT and GPT. A brief outline of IR, UV, NMR, Mass spectroscopy as tools for kinetic study.

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 ed., 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.
5. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint.2003, Pearson Education Pvt. Ltd., New Delhi.
6. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.
7. Instrumental Methods of Analysis by H.H. Willard, L.L. Merritt and J.A. Dean, 7th Edition, (1988).

8. Principles of instrumental analysis. D.A. Skoog, D.M. West, Holler, Nieman
9. Introduction to instrumental methods of analysis. D. Braun.
10. Principles and practice of analytical chemistry. Fifield and Kealey.
11. H.H.Bauer, G.D. Christien, and J.E.O'Reilly, eds., Instrumental analysis. Boston:Allyl and Bacon, 1978, Chapter 18, "Kinetic methods" by H.B. Mark, Jr.
12. R.A. Greinke and H.B.Mark, Jr., "Kinetic Aspects of Analytical Chemistry". Anal. chem., **46** (1974) 413 R.
13. H. L. Pardue, " A Comprehensive Classification of Kinetic Methods of Analysis used in Clinical Chemistry". Clin. Chem., **23**, (1977) 2189.
14. D. Perez-Bendito and M. Silva, Kinetic methods in analytical chemistry. New York: Wiley, 1988.
15. H.A. Mottola, Kinetic Aspects of Analytical Chemistry. New York: Wiley interscience, 1988.
16. H.U. Bergmeyer, Methods of Enzymatic Analysis, 3rd ed. New York: Wiley. A series of volumes plus index volume, 1983-1987

SOFT CORE PAPERS

CHA SCT 4.1 AUTOMATED AND METHODS OF CHEMICAL ANALYSIS

Objectives:

- To understand the instrumentation and applications of automated methods of analysis.
- To familiarize with analysis of real samples and clinical analysis.

Course outcome:

- Understand various types of automated methods of analysis.
- Identify activities that can be fully or partially automated.
- Automated chemical analysis will be very helpful in the clinical as well as pharmaceutical field to perform the purity analysis of the sample, although the sample size is very small, expensive and fast analysis.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animations are used in class room teaching.
- Students will be assigned numerical problems to understand the concepts.

Course content

UNIT-I

[16 HOURS]

Automated methods of analysis: An overview, definition, distinction between automatic and automated systems, advantages and disadvantages by automation, types of automated techniques. Nondiscrete techniques, segmented flow methods and basic equipment, special techniques and devices, theoretical considerations and problems, applications. Single channel and multi channel auto analysers, BUN analyzers, automatic glucose analyzers and ammonia in water analyzers, COD analyzers, CFA in industry. Non-segmented flow methods: Flow injection analysis. Principles, types of dispersion, factors affecting dispersion, applications of small, medium and large dispersions. Stopped flow methods, flow injection titrations. Discrete methods: Centrifugal fast scan analyzer, automatic multipurpose analyzers, Automatic elemental analyzer, automated analyzer based on multi layer film-principles, film structure, instrumentation applications. Comparison of discrete and non-discrete methods. Advantages of flow injection measurements over continuous flow measurements.

UNIT-II

[16 HOURS]

Analysis of real samples-real sample, choice of analytical method-defining the problem, investigating the literature, choosing or devising a method, testing the procedure, analysis of standard samples, using other methods, standard addition to the sample. Accuracy in the analysis of complex materials.

Decomposing and dissolving the sample- sources of error in decomposing and dissolution. Decomposing samples with inorganic acids. Microwave decomposition. Combustion methods for decomposing organic samples. Decomposition of inorganic materials with fluxes.

Clinical Analysis- Introduction, features of chinical analysis. Composition of blood, collection and preservation of samples. Common determinations - serum electrolytes, blood glucose and blood urea nitrogen, uric acid, albumin and globulins, acid and alkaline phosphates, barbiturates, chloride, sodium and potassium, bicarbonate, serum creatinine and cholesterol. Urine analysis- Principle components. Sample collection and preservation. Determination of creatinine, chloride, uric acid, ammonia, ascorbic acid, bilirubin and calcium.

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 ed., 2001 John Wiley & Sons, Inc, India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition,1993 prenticeHall, 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 Inidan Reprint.2003 PearsonEducation 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. Fifield and Kealey.
7. Instant Notes of Analytical Chemistry, Kealey and Haines, Viva Books Pvt. Ltd.,2002

CHI SCT: 4.2. BIOINORGANIC PHOTOCHEMISTRY

Objectives:

- To understand the photochemistry of inorganic compounds.
- To familiarize with the applications of fluorescents and chromogenic sensing and labeling.
- To learn photodynamic inactivation of microorganisms.

Course outcome:

- Basic concepts of photochemistry and photochemical reactions.
- Understand many organometallic compounds as fluroscent agents in the detection of cations, anions and toxic ions in the living system.
- Theory of photodynamics, and photocatalysis.

Pedagogy:

- Conventional method such as black board and chalk is used.

- Modern methods like power point presentation and animations are used in class room teaching.

Course content

UNIT-I

[16 HOURS]

Introduction, Philosophy of bioinorganic photochemistry

Fundamentals: Light and matter. Nature of light, Accessible light sources and Interaction between light and matter.

Formation and properties of electronic excited states: Wave mechanics and quantum numbers and Electronic excitation.

Photophysical deactivation of electronic excited states: Spontaneous deactivation, Quenching and Coordination and organometallic compounds.

Photochemical reactions: Photochemical reaction channels, Intramolecular photoreactions, Photodissociation and photoionization, Photoisomerization, Intermolecular photoreactions, the coordination compound specificity. Ligand field photochemistry, Photochemistry from LC or LLCT states, Inner-sphere charge transfer photochemistry, Outer-sphere charge transfer photochemistry, Photosensitized reactions, Homogeneous photocatalysis.

Natural photo-processes involving inorganic compounds

From interstellar space to planetary atmospheres: Homogeneous systems: from interstellar space to planetary atmospheres and primitive soup models. Heterogeneous photochemistry in ice phases.

UNIT-II

[16 HOURS]

Applications: Fluorescent and chromogenic sensing and labeling: Cations as targets in biochemical sensing Cations common in biological systems, Fluorescent detection of toxic cations, Fluorescent and chromogenic sensing of anions, Common anions and Toxic anions. Optical detection of neutral molecules. Nanoparticles in biochemical sensing and labeling.

Therapeutic strategies; Photobio-stimulation, Photo-activation of drugs, Photodynamic therapy, Mechanisms of PDT and PTT. Photosensitizers, Inorganic photosensitizers, Supporting role of metal ions in photodynamic therapy, and Combination of polypyrrolic photosensitizers and metallo-pharmaceuticals, Recent PDT development and Nanomedical methods.

Photodynamic inactivation of microorganisms: Bacteria, Viruses, Fungi and Parasites.

Phototoxicity and photoprotection: Chemical and physical photoprotection. Inorganic sunscreens.

Photocatalysis in environmental protection: Development of homo- and heterogeneous methods. Homogeneous photocatalysis and heterogeneous photocatalysis. Water and air detoxification. Other applications of photocatalysis.

References

1. Bioinorganic Photochemistry- Grazyna Stochel, Malgorzata Brindell, Wojciech Macyk, Zofia Stasicka, Konrad Szacilowski. Wiley Publishers (2009).
2. Photochemistry and Photophysics of Coordination Compounds I-Volume Editors: Balzani, V., Campagna, Springer Publications.Vol.280, 2007.
3. Photochemistry and Photophysics of Coordination Compounds II - Volume Editors: Balzani, V., Campagna, Springer Publications.Vol.281, 2007.

CHO SCT: 4.3. MEDICINAL CHEMISTRY

Objectives:

- To familiarize with the methods of isolation, structural elucidation and synthesis of carotenoids and vitamins.
- To learn the basics of medicinal chemistry.
- To understand the synthesis and applications of synthetic drugs.

Course outcome:

- To acquire the knowledge of biological significances of Carotenoids and vitamins.
- Understand the pharmacodynamics, pharmacokinetics and chemotherapy of several drugs.
- Synthesis and mechanism of drug actions of antimalarial, anticancer agents and cardiovascular drugs.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animations are used in class room teaching.

Course content

UNIT-I

[16 HOURS]

Carotenoids: Methods of isolation. Structure elucidation and synthesis of β-carotene. Structural relationship of α-, β- and γ-carotenes.

Vitamins: Introduction, constitution, synthesis and biological significance of thiamine, riboflavin, pyridoxine, biotin, ascorbic acid, vitamin A_1 & A_2, E_1 and E_2 , B_{12} and K groups.

UNIT-II

[16 HOURS]

Medicinal chemistry: Introduction, pharmacodynamics, pharmacokinetics, chemotherapy, metabolites antimetabolites, agonists and antiagonists. Classification drugs on the basis of therapeutic action. Concept of pro drug and soft drug. Theories of drug activity: Occupancy theory, rate theory, induced fit theory, concept of drug receptors. Evaluation methods: Free-wilson analysis, Hansch-anlysis, ID_{50} and IC_{50} (mathematical derivation of equation excluded).

Antipyretics: Aspirin, paracetamol, phenacetin, novalgin and their mechanism of action.

Antimalarials: structure, synthesis and mechanism of action of quinine and chloroquine.

Hypnotics: Analgesics and sedatives: phenoborbitol, chlordiazepoxide, meprobamate.

Stimulants: structure, action and synthesis of caffeine.

Antineoplastics: Structure, pharmacological action and synthesis of 5-flurouracil, chlorambucil, cyclophosphaminde and podophyllotoxin.

Cardiovascular drugs: Introduction, synthesis of dithiazem, verapamil, methyldopa, atenolol and oxprenolol.

References

1. Organic Chemistry, VI edition, Robert T. Morrison, Robert N. Boyd.
2. Organic Chemistry, Vol-II by I. L. Finar.
3. A text book of synthetic drugs, O. D. Tyagi and M. Yadav.
4. Synthetic drugs, Gurdeep R. Chatwal.
5. Medicinal chemistry by Graham Patrick.

CHP SCT: 4.4. QUANTUM CHEMISTRY AND BIOSENSORS

Objectives:

- To understand the applications of quantum mechanics to HMO theory.
- To learn the basics of biosensors and their applications.

Course outcome:

- Applications of quantum chemical methods in the theoretical evaluation of energies of molecules and reactions.
- Development of chemical and biochemical sensors and their applications in the determination of biomolecules.

Pedagogy:

- Conventional method such as black board and chalk is used.
- Modern methods like power point presentation and animations are also used in class room teaching.
- Students will be assigned to solve the numerical problems.

Course content

UNIT-I

16 HOURS]

Applications of quantum mechanics: Variation theorem: Statement and proof, application of variation theorem to a particle in one dimensional box, linear oscillator, H and He-atoms. Molecular orbital theory, LCAO-MO approximation, application to hydrogen molecule ion (H^{2+}), energy levels of H^{2+}, bonding and antibonding molecular orbitals, energy distribution, potential energy diagrams. Valence bond theory (VB), theory of H_2 molecule, Heitler-London method, energy levels, various modifications of Heitler-London wave function. Comparison of MO and VB theories. SCF method for many electron atom. Slater Orbitals –Effective nuclear charge (ENC), expressions for slater orbitals for 1s, 2s, 3s, 2p and 3d electrons (no derivation), Slater's rules for calculation of ENC. Theories of valence – Introduction, linear and non-linear variation functions, secular equations, coulombic, exchange, normalization and overlap integrals, secular determinants.

Huckel molecular orbital theory: Outline of method, assumptions. Application to ethylene, allyl radical, cyclopropenyl radical, butadiene, cyclobutadine, bicyclobutadine and benzene. Calculation of delocalization energy, charge density, π-mobile bond order and free valence.

UNIT-II

[16 HOURS]

Biosensors: Introduction, electrochemical biosensors: Amperometric, potentiometric and conductometric biosensors. Optical based biosensors: Surface plasma resonance, chemiluminesence, fibre optic biosensors, piozoelectronic sensors, mass selective and thermal sensors. Bio-recognition elements in biosensors, immobilization methods, principles of biorecognition, natural, semi-synthetic and synthetic biorecognition elements. Metabolism sensors: Glucose sensors, galactose sensors. Determination alcohol, ascorbic acid, D-isocitrate, oxalate, oxaloacetate, nitrite, nitrate, corbon monoxide, glycerol, triglycerides and sucrose. Biosensors using coupled enzyme reactions.

Applications of biosensors: Determination of glucose in blood, survey of biosensor methods for the determination of glucose. Determination of copper (I) in water using anodic stripping voltammetry.

References

1. Introductory Quantum Chemistry – A.K. Chandra. Second Edition, Tata McGraw Hill Publishing Co. Ltd., (1983).
2. Quantum Chemistry – Eyring, Walter and Kimball. John Wiley and Sons, Inc., New York.
3. Quantum Chemistry –I.N. Levine. Pearson Education, New Delhi, (2000).
4. Theoretical Chemistry – S. Glasstone. East West Press, New Delhi, (1973).
5. Quantum Chemistry – R.K. Prasad, New Age International Publishers, (1996).
6. Valence Theory – Tedder, Murel and Kettle.
7. Surface chemistry: Theory and applications, J. J. Bikertman, Academic press, New York (1972).
8. Chemical Kinetics, K. J. Laidler 3rd Edn., Harper International Edn., (1087).
9. Test Bok of Physical Chemistry, S. Glasston, McMillan India Ltd., 2nd Edn. (1986).
10. Physics at Surfaces, A. Zangwill, Combridge University Press (1988).
11. Surface Crystallography, L. J. Clarke, Wiley-Interscience (1985).
12. Biosensors: Fundamentals and Applications, Bansi Dhar Malhotra and Chandra Mouli Pandey, Smither Group Co., 2017, UK.
13. Biosensors: Techniques and Instrumentations in Analytical Chemistry, Frieder Scheller and Florian Schubert, Vol. 11, Elsevier Sci. Publishers, 1992.
14. Chemical Sensors and Biosensors, Brian R. Eggins, John Wiley & Sons Ltd, UK, 2004.

***