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UNIVERSITY OF MYSORE

Estd. 1916

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No.AC.2(S)/401/13-14

Dated: 24-05-2014

NOTIFICATION

Sub: Restructuring the Curriculum of Chemistry (PG) programme.

Ref: 1. Proceedings of Faculty of Science & Technology Meeting held on14-02-2014.
2. Proceedings of the Meeting of Academic Council held on 29-03-2014.

The Board of Studies in **Chemistry (PG)** at its meeting held on 02-12-2013 has resolved to restructuring the existing syllabus of Chemistry (PG) to be effective from the academic year 2014-15 onwards.

The Faculty of Science and Technology and the Academic Council at their meetings held on 14-02-2014.and 29-03-2014 respectively approved the above proposals and the same is hereby notified.

The copy of restructuring the existing syllabus of Chemistry (PG) is annexed herewith.

for S. Sampath 26/5/2014
REGISTRAR.
REGISTRAR
University of Mysore
MYSORE.

To

1. The Registrar (Evaluation), University of Mysore, Mysore.
2. The Chairperson, BOS/DOS in Chemistry, MGM.
3. The Dean, Faculty of Science & Technology, DOS in Zoology, MGM.
4. The Principals of the Affiliated Science Colleges.
5. The Deputy/Assistant Registrar (Evaluation), University of Mysore, Mysore.
6. Sri Narasimha Murthy, Statistician, E.B. UOM, Mysore.
7. The Supdt AC.1 & AC.2, A.B., Academic Section / PMEB, UOM., Mysore.
8. The P.A. to the Vice-Chancellor/Registrar/Registrar(Evaluation), UOM., Mysore.
9. The Case Worker, AC.7, Academic Section, University of Mysore, Mysore.
10. The Section Guard File(Supdt.AC.2), A.B., A.C., UOM.
11. The Schedule File.

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.
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 a minimum of 20 credits in Soft Core (sum total of 4 semesters) and 04 credits in Open Elective (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 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. Composite course means which includes both Theory and Practical.
3. HC: Hard Core; SC: Soft Core; OE: Open Elective

GENERAL SCHEME WITH RESPECT TO ASSESSMENT OF CREDITS

Semester	Hard Core		Soft Core		Open Elective
I Semester	**I**	2 + 0 + 2 = 4	**A**	2 + 0 + 2 = 4[a]	--
	O	2 + 0 + 2 = 4	**I**	2 + 0 + 0 = 2	
	P	2 + 0 + 2 = 4	**O**	2 + 0 + 0 = 2	
	G	3 + 0 + 0 = 3	**P**	2 + 0 + 0 = 2	
II Semester	**I**	2 + 0 + 2 = 4	**A**	2 + 0 + 2 = 4[a]	3 + 1 + 0 = 4[b] (General Chemistry)
	O	2 + 0 + 2 = 4	**I**	2 + 0 + 0 = 2	
	P	2 + 0 + 2 = 4	**O**	2 + 0 + 0 = 2	3 + 1 + 0 = 4[b] (Chemistry)
	G	3 + 0 + 0 = 3	**P**	2 + 0 + 0 = 2	
III Semester	**I**	3 + 0 + 0 = 3	**A**[c]	2 + 0 + 2 = 4[d]; 2 + 0 + 0 = 2	3 + 1 + 0 = 4[b] (General Chemistry)
	O	3 + 0 + 0 = 3	**I**[c]	2 + 0 + 2 = 4[d]; 2 + 0 + 0 = 2[d]	
	P	3 + 0 + 0 = 3	**O**[c]	2 + 0 + 2 = 4[d]; 2 + 0 + 0 = 2[d]	3 + 1 + 0 = 4[b] (Chemistry)
	--		**P**[c]	2 + 0 + 2 = 4[d]; 2 + 0 + 0 = 2[d]	
IV Semester	**I**	3 + 0 + 0 = 3	**A**[c]	2 + 0 + 2 = 4[d]; 2 + 0 + 0 = 2	--
	O	3 + 0 + 0 = 3	**I**[c]	2 + 0 + 2 = 4[d]; 2 + 0 + 0 = 2[d]	
	P	3 + 0 + 0 = 3	**O**[c]	2 + 0 + 2 = 4[d]; 2 + 0 + 0 = 2[d]	
	Diss.	4 + 0 + 0 = 4	**P**[c]	2 + 0 + 2 = 4[d]; 2 + 0 + 0 = 2[d]	
Total Credits	**52**		**20 (46)**		**04 (08)**

Note:
A – Analytical; I – Inorganic; O – Organic; P – Physical; G - General Chemistry; Diss. – Dissertation/Project work
e.g., X + Y + Z: Theory + Tutorial + Practical

[a] All students have to opt composite paper (Theory + Practical) in Soft Core compulsorily in both I and II Semesters

[b] Courses are common for both II and III Semesters and it is only for non-chemistry students

[c] Among the strength in class, each 25% is allowed to opt one composite paper (Theory + Practical) in both III and IV Semesters since it is very difficult to accommodate all the students in any one branch

[d] Courses are common for both III and IV Semesters

SCHEME OF STUDY AND EXAMINATION
FIRST SEMESTER

HARD CORE

Courses	Title	Contact Hours/ week	Credit	Max. Marks	Internal Assessment Marks		Semester End Exams (C_3)	
					C_1	C_2	Duration	Max. Marks
CHI HCT: 1.1.	Concepts and Models of Inorganic Chemistry + Inorganic Chemistry Practicals-I	02+04	04	100	15	15	03	70
CHO HCT: 1.2.	Reaction Mechanism + Organic Chemistry Practicals-I	02+04	04	100	15	15	03	70
CHP HCT: 1.3.	Physical Chemistry-I + Physical Chemistry Practicals-I	02+04	04	100	15	15	03	70
CHG HCT: 1.4.	Symmetry, Group Theory and Chemical Spectroscopy	03	03	100	15	15	03	70

Note: For all Composite Courses, Theory will be evaluated for 100 marks and Practical for 100 marks separately and the average will be taken for the result declaration.

SOFT CORE

Courses	Title	Contact Hours/ week	Credit	Max. Marks	Internal Assessment Marks		Semester End Exams (C_3)	
					C_1	C_2	Duration	Max. Marks
CHA SCT: 1.51.	Fundamentals of Chemical Analysis + Analytical Chemistry Practicals-I	02+04	04	100	15	15	03	70
CHI SCT: 1.52.	Chemistry of Selected Elements	02	02	100	15	15	03	70
CHO SCT: 1.53.	Vitamins and Medicinal Chemistry	02	02	100	15	15	03	70
CHP SCT: 1.54.	Biophysical Chemistry and Pharmacokinetics	02	02	100	15	15	03	70

SECOND SEMESTER
HARD CORE

Courses	Title	Contact Hours/ week	Credit	Max. Marks	Internal Assessment Marks		Semester End Exams (C_3)	
					C_1	C_2	Duration	Max. Marks
CHI HCT: 2.1.	Coordination Chemistry + Inorganic Chemistry Practicals-II	02+04	04	100	15	15	03	70
CHO HCT: 2.2.	Stereochemistry and Heterocyclic Chemistry + Organic Chemistry Practicals-II	02+04	04	100	15	15	03	70
CHP HCT: 2.3.	Physical Chemistry-II + Physical Chemistry Practicals-II	02+04	04	100	15	15	03	70
CHG HCT: 2.4.	Molecular Spectroscopy-II	03	03	100	15	15	03	70

SOFT CORE

Courses	Title	Contact Hours/ week	Credit	Max. Marks	Internal Assessment Marks		Semester End Exams (C_3)	
					C_1	C_2	Duration	Max. Marks
CHA SCT: 2.51.	Separation Techniques + Analytical Chemistry Practicals-II	02+04	04	100	15	15	03	70
CHI SCT: 2.52.	Industrial Inorganic Chemistry	02	02	100	15	15	03	70
CHO SCT: 2.53.	Dyes and Insecticides	02	02	100	15	15	03	70
CHP SCT: 2.54.	Nanomaterials, Semiconductors and Superconductors	02	02	100	15	15	03	70

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	Max. Marks
CH OET: 2.1/3.1.	Chemistry	04	04	100	15	15	03	70
CH OET: 2.2/3.2.	General Chemistry	04	04	100	15	15	03	70

Note: Each course will have three units and one tutorial class/week

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	Max. Marks
CHI HCT: 3.1.	Advanced Inorganic Chemistry	03	03	100	15	15	03	70
CHO HCT: 3.2.	Reagents in Organic Synthesis	03	03	100	15	15	03	70
CHP HCT: 3.3.	Physical Chemistry-III	03	03	100	15	15	03	70

SOFT CORE

COMPOSITE

Courses	Title	Contact Hours/ week	Credit	Max. Marks	Internal Assessment Marks		Semester End Exams (C_3)	
					C_1	C_2	Duration	Max. Marks
CHA SCT: 3.41.	Applied Analysis I + Analytical Chemistry Practicals-III	02+04	04	100	15	15	03	70
CHI SCT: 3.42.	Frontiers in Inorganic Chemistry + Inorganic Chemistry Practicals- II	02+04	04	100	15	15	03	70
CHO SCT: 3.43.	Carbohydrates, Proteins and Nucleic Acids + Organic Chemistry Practicals-III	02+04	04	100	15	15	03	70
CHP SCT: 3.44.	Applications of Electrochemistry and Corrosion + Physical Chemistry Practicals-III	02+04	04	100	15	15	03	70

NON-COMPOSITE

Courses	Title	Contact Hours/ week	Credit	Max. Marks	Internal Assessment Marks		Semester End Exams (C_3)	
					C_1	C_2	Duration	Max. Marks
CHI SCT: 3.42.	Bioinorganic Photo chemistry	02	02	100	15	15	06	50
CHOSCT: 3.52.	Lipids, Porphyrins, Anthocyanins and Flavonoids	02	02	100	15	15	06	50
CHP SCT: 3.53.	Applications of X-ray crystallography and Quantum Chemistry	02	02	100	15	15	06	50

OPEN ELECTIVE

All the courses are same as that described 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	Max. Marks
CHI HCT: 4.1.	Bioinorganic Chemistry	03	03	100	15	15	03	70
CHO HCT: 4.2.	Photochemistry, Pericyclic Reactions and Organometallic Chemistry	03	03	100	15	15	03	70
CHP HCT: 4.3.	Physical Chemistry-IV	03	03	100	15	15	03	70

SOFT CORE

All the courses are same as that described in III 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 both HC/SC/OE as well as Composite and Non-composite courses' assessment of marks.

The following is the scheme which will be followed for the assessment of marks for HC/SC/OE as well as Composite and Non-composite courses irrespective of the credits associated with each course. 30% of the marks will be assessed for the 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. The distribution of marks for C_1 and C_2 varies with HC and SC courses.

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	Internal Assessment Marks
C_2 Component	: 15 Marks	
C_3 Component	: 70 Marks	Semester End Examination
Total	**: 100 Marks**	

The above will be followed in common for all the HC/ SC (Composite/ Non-composite)/ OE courses in all the four semesters.

1. HARD CORE (03 CREDIT COURSES)/ OPEN ELECTIVE (04 CREDIT COURSES)

1.1. 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, Home Assignment and Seminar***. 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. Home Assignment will be concerned for C_1 Component and Seminar for C_2 Component only. Hence, a teacher may give only one assignment (or in their personal interest one more may be given). Since each course has three units, the marks shall be divided equally. Allotment of marks for C_1 and C_2 is as follows: Out of 15 Marks for IA 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). IA 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 assigned for 05 Marks for the favor of IA. Please note that actual Seminar will be assessed for 20 Marks and finally 05 Marks will be distributed to each theory HC course. i.e.,

C_1		**C_2**	
Internal Test	: 30 Marks (10+10+10) **Reduced to 10 Marks**	Internal Test	: 30 Marks (10+10+10) **Reduced to 10 Marks**
Home Assignment	: 15 Marks (05+05+05) **Reduced to 05 Marks**	Seminar	: 20 Marks (05+05+05+05) **Distributed 05 Marks to each HC course**
Total	**: 15 Marks**	**Total**	**: 15 Marks**

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

The question paper is of 3 hr duration with Max. Marks 70. The following question paper pattern will be followed for all the theory courses (HC/SC/OE). Question paper will have 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 (5+5+4) 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.*

1. Nine Medium/ Short Answer Type Questions and any seven should be answered. Each question carries TWO marks. **[7 x 2 = 14]**
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 (5+5+4) 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 x 14 = 56]**

   a.
   b.
   c.
   or
   c.

2. HARD CORE/ SOFT CORE (04 CREDIT COURSES)

Those course which have 04 credits under HC or SC are called by '**Composite Course**' which means that a course which contains both Theory as well as Practical components. However, evaluation will be done on the following basis. Both Theory and

Practical will be assessed for 100 marks separately (which includes $C_1+C_2+C_3$) and an average from these two will be taken for the result declaration. The assessment pattern discussed above in 1 holds good here also. For the Practical assessment please refer '**4. Practicals**' below.

3. SOFT CORE (02 CREDIT COURSES)

3.1. Distribution of Marks for C_1 and C_2 Components

IA consists of 25 marks; it will be divided into two parts viz., ***Internal Test and Home Assignment***. Internal tests will be conducted during the 8th week of the semester for C_1 and 16th 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**

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

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

4. PRACTICALS

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

Each practical (HC/SC) 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 (HC/SC) 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**	

4.1. 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**

4.2. 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**

5. DISSERTATION/ PROJECT WORK (04 CREDIT COURSE)

Each student is expected to undergo Dissertation/ Project Work under the guidance of the faculty of the department during the IV Semester.

5.1. Distribution of Marks for C_1 and C_2 Components

IA consists of **15 Marks**; it will be divided into three parts viz., ***Attendance, Continuous Assessment and Work Progress***. Continuous assessment refers to the daily assessment of each student based on his or her skill, results obtained, literature survey etc. C_1 will be assessed during the 8th week of the semester and C_2 during the 16th week of the semester. Hence, the concerned guide will prepare the marks list based on the above said parameters for both C_1 and C_2 Components.

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

The end examination will be conducted for **70 Marks**. Every student is suppose to prepare a hard copy of the findings of the work in the form of dissertation and submitted for evaluation. This part will be assessed for 50 Marks. Each student will be subjected to Viva-Voce Examination for which 20 Marks is allotted. i.e.,

Evaluation of Dissertation	: 50 Marks
Viva-Voce	: 20 Marks
Total	**: 70 Marks**

FIRST SEMESTER

CHI HCT: 1.1. CONCEPTS AND MODELS OF INORGANIC CHEMISTRY

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 and cadmium iodide) types. The perovskite and spinel structures. Thermodynamics of ionic crystal formation. Lattice energy, Born-Haber cycle, Born-Lande equation. Applications of lattice energetics. Radius ratio rules

Structures and energetics of inorganic molecules: Introduction, Energetics of hybridization. VSEPR model for explaining structure of AB, AB_2E, AB_3E, AB_2E_2, ABE_3, AB_2E_3, AB_4E_2, AB_5E and AB_6 molecules. M.O. treatment of homonuclear 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 and HF) aprotic solvents (liquid SO_2, BrF_3 and N_2O_4). Solutions of metals in liquid ammonia, hydrated electron. Super acids.

Inner transition elements: Spectral and magnetic properties, redox chemistry.

Applications: Lanthanides as shift reagents, high temperature super conductors. Chemistry of trans-uranium elements.

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, 3rd edition. G.L. Miessler and D.A. Tarr, Pearson Education (2004).
4. Inorganic Chemistry, 2nd edition. D.F. Shriver, P.W. Atkins and C.H. Langford, Oxford University Press (1994).

5. Inorganic Chemistry, 2nd edition. C.E. Housecroft and A.G. Sharpe, Pearson Education Ltd. (2005).
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).

INORGANIC CHEMISTRY PRACTICALS – I

[64 HOURS]

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

References

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

CHO HCT: 1.2. REACTION MECHANISM

UNIT – I

[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.

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

UNIT – II

[16 HOURS]

Substitution reactions – Kinetics, mechanism and stereochemical factor affecting the rate of S_N^1, S_N^2, S_{RN}^i, S_N^i, $S_N^{1'}$, $S_N^{2'}$, S_N^{1i} and SRN^1 reactions, Neighbouring group participation.

Electrophilic substitution reactions – Kinetics, mechanism and stereochemical factor affecting the rate of S_E1 & S_E2

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 - E1, E2, E1cB. cis elimination, Hofmann and Saytzeff eliminations, competition between elimination and substitution, decarboxylation reactions. Chugaev reaction.

References

1. H. Pine, Hendrickson, Cram and Hammond, Organic Chemistry, Mc Graw Hill, New York, 1987.
2. I.L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
3. N.S. Issacs, Reactive Intermediates in Organic Chemistry, John Wiley and Sons, New York.1974.
4. R.K. Bansal, Organic Reaction Mechanism, Wiley Eastern Limited, New Delhi, 1993.
5. J. March, Advanced Organic Chemistry, Wiley Interscience, 1994.
6. A Guide Book to Mechanism in Organic Chemistry by Petersykes.
7. F.A. Carey and Sundberg, Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York, 1990.
8. S.K. Ghosh, Advanced General Organic Chemistry, Book and Alleied (P) Ltd, 1998.

ORGANIC CHEMISTRY PRACTICALS – I

[64 HOURS]

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

References

1. Manual of Organic Chemistry - Dey and Seetharaman.
2. Modern Experimental Organic Chemistry by John H. Miller and E.F. Neugil, p 289.
3. An Introduction to Practical Organic Chemistry - Robert, Wingrove etc.
4. A Text Book of Practical Organic Chemistry – A.I. Vogel, Vol. III.
5. Practical Organic Chemistry - Mann & Saunders.

6. Semimicro Qualitative Organic Analysis by Cheronis, Entrikin and Hodnet.

CHP HCT: 1.3. PHYSICAL CHEMISTRY – I

UNIT – I

[16 HOURS]

Concepts of entropy and free energy: A brief resume of laws of thermodynamics (First and second laws). Entropy as a measure of unavailable energy. Entropy change during spontaneous process. Helmholtz and Gibbs free energies. Thermodynamic criteria of equilibrium and spontaneity. Variation of free energy with temperature and pressure. Maxwell's relations. Third law of thermodynamics - calculation of absolute entropies. Nernst heat theorem & its applications.

Partial molar properties: Partial molar volumes and their determination 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: Concept of fugacity, Determination of fugacity of gases. Variation of fugacity with temperature and pressure. Activity and activity coefficients. Variation of activity with temperature and pressure. Determination of activity co-efficients by vapour pressure, depression in freezing point, solubility measurements by electrical methods.

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

UNIT – II

[16 HOURS]

Chemical Kinetics: Determination of order of reactions, complex reactions - parallel, consecutive and reversible reactions. Chain reactions - Branched chain reactions- general rate expression, 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 of unimolecular reactions. Qualitative account of its modifications (no derivation).

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

Reactions in solution: Ionic reactions - salt and solvent effects. Effect of pressure on the rates of reactions. Cage effect with an example. Oscillatory reactions.

Fast reactions- 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.

Reference

1. Physical Chemistry by P.W. Atkins, ELBS, 5th edition, Oxford University Press (1995).

2. Text Book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2nd edition (1974).
3. Elements of Physical Chemistry by Lewis and Glasstone.
4. Fundamentals of physical chemistry – Maron and Lando (Collier Macmillan) 1974.
5. Thermodynamics for Chemists by S. Glasstone, Affiliated East-West Press, New Delhi, (1965).
6. Chemical Thermodynamics by I.M. Klotz, W.A. Benzamin Inc. New York, Amsterdam (1964).
7. Chemical Kinetics by K.J. Laidler.
8. Chemical Kinetics by Frost and Pearson.
9. Kinetics and Mechanism of Chemical Transformation by J. Rajaram and J.C. Kuriacose.
10. Chemical Kinetics by L.K. Jain.
11. Chemical Kinetics by Benson.

PHYSICAL CHEMISTRY PRACTICALS – I

[64 HOURS]

1. Study of kinetics of hydrolysis of an ester using HCl/H_2SO_4 at two different temperatures, determination of rate constants and energy of activation.
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, determination of rate constant.
4. Conductometric titration of a mixture of HCl and CH_3COOH against NaOH.
5. Conductometric titration of sodium sulphate against barium chloride.
6. Determination of equivalent conductance at infinite dilution of a strong electrolytes and verification of Onsager equation.
7. Potentiometric titration of KI *vs* $KMnO_4$ solution.
8. Determination of dissociation constant of a weak acid by potentiometric method.
9. Potentiometric titration of $AgNO_3$ *vs* KCl.
10. To obtain the absorption spectra of coloured complexes, verification of Beer's law and estimation of metal ions in solution using a spectrophotometer.
11. Spectrophotometric titration of $FeSO_4$ against $KMnO_4$.
12. Determination of heat of solution of benzoic acid by variable temperature method (graphical method).
13. 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.
14. Determination of the molecular weight of a polymer material by viscosity measurements (cellulose acetate/methyl acrylate).
15. Analysis of a binary mixture (Gylcerol & Water) by measurement of refractive index.

16. Determination of degree of association of benzoic acid in benzene by distribution method.

Reference

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.

CHG HCT: 1.4. SYMMETRY, GROUP THEORY AND CHEMICAL SPECTROSCOPY

UNIT – I

[16 HOURS]

Molecular symmetry and group theory: Symmetry elements and symmetry operations. Concept of a group, definition of a point group. Classification of molecules into point groups. Subgroups. Schoenflies and Hermann-Maugin symbols for point groups. Multiplication tables (C_n, C_{2V} 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 orbital. Group theory to Crystal field theory and Molecular orbital theory (octahedral and tetrahedral complexes). Determining the symmetry groups of normal modes (both linear and non-linear molecules).

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. Relative intensities of the spectral lines. Classification of polyatomic molecules based on moment of inertia - Linear, symmetric top, asymmetric top and spherical molecules. Rotation spectra of polyatomic molecules (OCS 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. Vibration - rotation spectra of carbon monoxide. Expressions for fundamental and overtone frequencies. Vibration of polyatomic molecules – The number of degrees of freedom of vibration. Parallel and perpendicular vibrations (CO_2 and H_2O). fundamental, overtone, combination and difference bands. Fermi resonance. Force constant and its significance. Theory of infrared absorption and theoretical group frequency. Intensity of absorption band and types of absorptions. Correlation chart. Important spectral regions - hydrogen stretching region, double and triple bonds regions, fingerprint region. Factors affecting the group frequency – Physical state, vibrational coupling, electrical effect, hydrogen bonding, steric effect and ring strain. Applications: Structures of small molecules: XY_2 – linear or bent, XY_3 – planar or pyramidal.

UNIT – III

[16 HOURS]

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

UV Visible spectroscopy: Quantitative aspects of absorption – Beer's law, Technology associated with absorption measurements. Limitations of the law – real, chemical, instrumental and personal. 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. 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. Applications: Qualitative and quantitative analysis of binary mixtures, measurements of dissociation constants of acids and bases, determination of molecular weight, determination of stoichiometry and stability of the complexes. Photometric titrations, kinetic studies.

References

1. Chemical Applications of Group Theory, 3rd edition, F.A. Cotton, John Wiley and Sons (2006).
2. Molecular Symmetry and Group Theory – Robert L Carter, John Wiley and Sons (2005).
3. Symmetry in Chemistry - H. Jaffe and M. Orchin, John Wiley, New York (1965).
4. Vibrational Spectroscopy - Theory and Applications- D.N. Sathyanarayana, New Age International Publications, New Delhi (1996).

5. Group Theory and its Chemical Applications - P.K. Bhattacharya, Himalaya Publications, New Delhi (1998).
6. Fundamentals of Molecular Spectroscopy, C.N. Banwell and E.M. McCash. 4th edition, Tata McGraw Hill, New Delhi.
7. Fundamentals of molecular spectroscopy, G. M. Barrow, MgGraw Hill, New York (International students Edition), 1974.
8. Theoretical chemistry, S. Glasstone, affiliated East-West Press Pvt. Ltd, New Delhi, 1973.
9. Introduction to Spectroscopy - Pavia, Lampman and Kriz, 3rd edition, Thomson.
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.
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, 7th Edition, 1988.
15. Physical methods in inorganic chemistry, R. S. Drago, affiliated East-West press Pvt. Ltd., (Student Edition) 1978.

CHA SCT: 1.51 FUNDAMENTALS OF CHEMICAL ANALYSIS

UNIT – I

[16 HOURS]

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

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

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

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 – II

[16 HOURS]

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.

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

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

References

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

ANALYTICAL CHEMISTRY PRACTICALS – I

[64 HOURS]

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 aspirin in their tablet preparations by residual acid-base titrimetry.
6. Determination of purity of aniline
7. Assay of chlorpromazine tablets by non-aqueous acid-base titration.
8. Determination of carbonate and bicarbonate in a mixture by *p*H-metric titration and comparison with visual acid-base titration.
9. Determination of benzoic acid in food products by titration with methanolic KOH in chloroform medium using thymol blue as indicator.
10. Analysis of water/waste water for acidity by visual, *p*H metric and conductometric titrations.
11. Analysis of water/waste water for alkalinity by visual, *p*H metric and conductometric titrations.
12. Determination of carbonate and hydroxide-analysis of a commercial washing soda by visual and *p*H-titrimetry.
13. Spectrophotometric determination of creatinine and phosphorus in urine.
14. Flame emission spectrometric determination of sodium and potassium in river/lake water.

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 SCT: 1.52 CHEMISTRY OF SELECTED ELEMENTS

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 liquid ammonia. Coordination and organometallic comopounds. Applications.
The Group 2 elements: Occurrence, extraction and uses. Halides, hydrides and salts of oxoacids. Complex ion in aqueous solution and complexes with amido and alkoxy ligands.
The Group 17 elements: Occurrence, recovery and uses. Trends in properties and pseudohalogens.

UNIT – II

[16 HOURS]

Interhalogens: Physical properties and structures, chemical properties, cationic interhalogens, halogen complexes and polyhalides.
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 Wiley and Sons (2002).
2. Inorganic Chemistry, 3rd edition. James E. Huheey, Harper and Row Publishers (1983).
3. Inorganic Chemistry, 3rd edition. G.L. Miessler and D.A. Tarr, Pearson Education (2004).
4. Inorganic Chemistry, 2nd edition. C.E. Housecroft and A.G. Sharpe, Pearson Education.
5. Chemistry of the Elements – N.N. Greenwood and A. Earnshaw, Pergamon Press (1985).
6. Inorganic Chemistry - 2nd edition, D.F. Shriver, P.W. Atkins and C.H. Langford, Oxford University Press, (1994).
7.

CHO SCT: 1.53 VITAMINS AND MEDICINAL CHEMISTRY

UNIT – I

[16 HOURS]

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

Green chemistry:

Definition and principles, planning a green synthesis in a chemical laboratory, Green preparation-Aqueous phase reactions, solid state (solvent less) reactions, photochemical reactions, Phase transfer catalyst catalyzed reactions, enzymatic transformations & reactions in ionic liquids.

UNIT – II

[16 HOURS]

Medicinal Chemistry-Chemotherapy: Definition, History, and Evolution of Chemother

Classification of drugs on the basis of therapeutic action, pharmacophonic, API (active pharmaceutical ingredient) chiral drugs, development of new drugs, procedures followed in drug design, concept of lead and lead-compounds and lead modifications, molecular modeling, concept of pro-drug and soft drug, factor affecting bioactivity.

Theories of drug activity, occupancy-theory, rate theory, induced-fit theory. Quantitative structure-activity relationship, history and development of QSAR, concept of drug receptors, elementary treatment of drug receptor interactions.

Physiochemical parameters: lipophilicity, partition-coefficient, electronic ionization constant, steric, Shelton and surface activity parameters and redox potential.

Evaluation methods: Free-Wilson analysis, Hansch-analysis, relationship between Free-Wilson analysis and Hansch-analysis – LD_{50}, ED_{50}, ID_{50}, IC_{50} (mathematical derivation of equation excluded).

References

1. Introduction to medicinal chemistry, A Gringuage, Wiley-VCH.
2. Wilson and Gisvold's Text Book of organic medicinal and pharmaceutical chemistry, Ed Robert F. Dorge.
3. An introduction to drug design, S.S. Pandey and J.R. Dimmock, New Age International.
4. Burger's medicinal chemistry and drug discovery, Vol-1 (Chapter-9 and Ch-14), Ed.M.E. Wolff, John Wiley.
5. L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
6. K. Albert, L. Lehninger, D. L. Nelson, M. M. Cox, Principles of Biochemistry, CBZ publishers, 1st edition, New Delhi, 1993.
7. Harper’s Biochemistry, Ed. R. Harper, 22^{nd} edition, Prentice Hall Press, New York, 1990.
8. Harper’s review of biochemistry – P. W. Martin, P. A. Mayer & V. W. Rodfwell, 5^{th} edition, Maurzen Asian Edition, California, 1981.

CHP SCT: 1.54. BIOPHYSICAL CHEMISTRY AND PHARMACOKINETICS

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. Electroosmosis and streaming potential and its biological significance. Biological significance of Donnan membrane phenomenon. Micelles and its involvement during digestion and absorption of dietary lipids. Diffusion of solutes across biomembranes and its application in the mechanism of respiratory exchange. "Salting In" and "Salting Out" of proteins. Osmotic behaviour of cells and osmo-regulation and its application in the evolution of excretory systems of organisms. Effect of temperature and *p*H on the viscosity of biomolecules (albumin solution). Significance of viscosity in biological systems - mechanism of muscle contraction, detection of intrastrand disulfide bonds in proteins, polymerization of DNA and nature of blood flow through different vessels. Effect of temperature, solute concentration (amino acids) on surface tension. Biological significance of surface tension - stability of Alveoli in lungs, interfacial tension in living cells (Danielli and Davson model). Application of sedimentation velocity and sedimentation equilibrium method for molecular weight determination of proteins.

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 (4^{th} 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

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.

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.

Reaction and Mechanisms: Introduction. Substitution reactions - Inert and labile compounds, mechanisms of substitution.

Kinetic consequences of Reaction pathways - Dissociation, interchange and association. Experimental evidence in octahedral substitution - Dissociation, associative mechanisms, the conjugate base mechanism, the kinetic chelate effect.

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

Electron-transfer processes: Inner-sphere mechanism and outer-sphere mechanism, conditions for high and low oxidation numbers. Photochemistry of Coordination Compounds: Overview and General Concepts.

References

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

INORGANIC CHEMISTRY PRACTICALS – II

[64 HOURS]

PART – I

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. Gravimetric determination of copper(II) and nickel(II) using salicylaldoxime.
4. Preparation of mercurytetrathiocyanatocobaltate(II) and estimation of mercury by gravimetry.
5. Preparation of tris(oxalato)ferrate(III) and estimate the metal ion.

PART – II

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

References

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

CHO HCT: 2.2. STEREOCHEMISTRY AND HETEROCYCLIC CHEMISTRY

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]

Nomenclature of heterocyclic compounds. Structure (no elucidation), reactivity, synthesis (minimum three synthesis) and reactions (minimum three reactions) of furan, pyrrole, thiophene, indole, pyridine, quinoline, isoquinoline, pyrazole, imidazole, pyrone, coumarin, chromones, pyrimidines, purines.

References

1. J. March, Advanced Organic Chemistry, Wiley Inter Science, 1994.
2. F.A. Carey and Sundberg, Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York, 1990.
3. Comprehensive Organic Synthesis – B.M. Trost and I. Fleming series, Pergamon Press, New York, 1991.
4. S.K. Ghosh, Advanced General Organic Chemistry, Book and Allied (P) Ltd., 1998.
5. Heterocyclic Chemistry – Joule & Smith.
6. Basic Principles of Heterocyclic Chemistry – L.A. Pacquette.
7. E.L. Eliel and S.H. Wilen, Stereochemistry of Organic Compounds, John Wiley and Sons, New York. 1994.
8. Stereochemistry and Mechanism through Solved Problems by P.S Kalsi.

ORGANIC CHEMISTRY PRACTICALS – II

[64 HOURS]

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 *via* cyclohexanone.
4. Esterification: Preparation of benzoccaine from *p*-nitrotoluene.
5. Diazotization (Sandmeyer's reaction): Preparation of *p*-chlorobenzoic acid from *p*-toluidine.
6. Molecular rearrangement: Preparation of *o*-chlorobenzoic acid from phthalic anhydride.
7. Preparation benzilic acid from benzaldehyde**.**
8. Preparation of *o*-hydroxy benzophenone from phenyl benzoate *via* Fries rearrangement.
9. Prepartion of benzanilide from benzophenone oxime *via* Beckmann rearrangement.
10. Synthesis of *m*-chloroiodobenzene from *m*-dinitrobenzene.

References

1. Manual of Organic Chemistry - Dey and Seetharaman.
2. Modern Experimental Organic Chemistry by John H. Miller and E.F. Neugil, p 289.
3. An Introduction to Practical Organic Chemistry - Robert, Wingrove etc.
4. A Text Book of Practical Organic Chemistry – A.I. Vogel, Vol.III.

5. Practical Organic Chemistry - Mann & Saunders.

CHP HCT: 2.3. PHYSICAL CHEMISTRY – II

UNIT – I

[16 HOURS]

Electrochemistry of solutions: Arrhenius theory of strong and weak electrolytes and its limitations. 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). Determination of transference number by emf and Hittorf's methods. True and apparent transference numbers. Abnormal transference numbers, effect of temperature on transference numbers. Liquid junction potential-determination and minimization.

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. Polarography- Half wave potential, application in qualitative and quantitative analysis. Butler-Volmer equation, Tafel equation. Hydrogen oxygen over voltage. Effect of temperature, current density and *p*H on over voltage.

UNIT – II

[16 HOURS]

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

Reference

1. Text Book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2nd edition (1974).
2. Elements of Physical Chemistry by Lewis and Glasstone.
3. Physical Chemistry by P.W. Atkins, ELBS, 4th edition, Oxford University Press (1990).
4. Physical Chemistry – G.M. Barrow, McGraw Hill International Service (1988).
5. Introduction to Electrochemistry by S. Glasstone.

6. Electrochemistry –Principles and Applications by E.G. Potter.
7. Electrochemistry by Reiger, Prentice Hall (1987).
8. Modern Electrochemistry Vol. I and II by J.O.M. Bockris and A.K.N. Reddy, Pentium Press, New York (1970).
9. Quantum Chemistry – A.K. Chandra. 2^{nd} edition, Tata McGraw Hill Publishing Co. Ltd., (1983).
10. Quantum Chemistry – Eyring, Walter and Kimball. John Wiley and Sons, Inc., New York.
11. Quantum Chemistry – I.N. Levine. Pearson Education, New Delhi, (2000).
12. Theoretical Chemistry – S. Glasstone. East West Press, New Delhi, (1973).
13. Quantum Chemistry – R.K. Prasad, New Age International Publishers, (1996).
14. Valence Theory – Tedder, Murel and Kettle.
15. Quantum Chemistry – D.A. McQuarrie.

PHYSICAL CHEMISTRY PRACTICALS – II

[64 HOURS]

1. Study of kinetics of reaction between CAT and indigocarmine spectrophotometrically and determination of rate constant.
2. Kinetics of reaction between sodium formate and iodine, determination of energy of activation.
3. Determination of energy of activation for the bromide-bromate reaction.
4. Determination of dissociation constant and mean ionic activity coefficient of weak electrolytes by conductivity method.
5. Conductometric titration of oxalic acid against NaOH and NH_4OH.
6. pH titration of (a) CH_3COOH vs. NaOH and determination of K_a.
7. Potentiometric titration of a mixture of halides (KCl+KI) against $AgNO_3$.
8. Determination of redox potential of Fe^{2+} ions by potentiometric method.
9. Determination of activity of 0.1 M HCl by EMF method.
10. Determination of partial molar volume of NaCl-H_2O/KCl- H_2O/KNO_3/ H_2O systems.
11. G.M. Counter – determination of G.M. plateau and dead time.
12. Verification of inverse square law using gamma emitter.
13. Determine the concentration of KI potentiometrically by calibration method.
14. To study the kinetics of reaction between acetone and iodine - determination of order of reaction w.r.t. iodine and acetone.
15. To determine the eutectic point of a two component system (Naphthalene-*m*-dinitrobenzene system).
16. Coulometric titration I_2 vs $Na_2S_2O_3$.

Reference

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.

CHG HCT: 2.4. MOLECULAR SPECTROSCOPY – II

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), variable temperature probe, FT-NMR, Spectroscopy and advantages. ^{13}C-NMR Spectroscopy: Comparison of ^{1}H-NMR and ^{13}C-NMR, multiplicity-Proton decoupling-Noise decoupling-Off resonance decoupling-Selective proton decoupling - Chemical shift, application of CMR. NMR of ^{19}F, ^{31}P, ^{11}B and ^{15}N Applications of NMR: Structural diagnosis, conformational analysis, keto-enol tautomerism, H bonding. Two dimensional NMR Spectroscopy: COSY, NOESY, MRI.

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: Quadrupolar nuclei, electric field gradient, nuclear quadrupole coupling constants, energies of quadrupolar transitions, effect of magnetic field. Applications. **Mössbauer spectroscopy**: The Mössbauer effect, chemical isomer shifts, quadrupole interactions, measurement techniques and spectrum display, application to the study of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+} compounds, nature of M-L bond, coordination number and structure), detection of oxidation states and inequivalent Mössbauer atoms.

UNIT – III

[16 HOURS]

IR spectroscopy: Introduction, instrumentation, sample handling, modes of vibrations, Hooks law, Characteristic group frequencies and skeletal frequencies. Finger print region, Identification of functional groups- alkenes, aromatics, carbonyl compounds (aldehydes and ketones, esters and lactones), halogen compounds, sulphur and 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 molecules.

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 SCT 2.51: SEPARATION TECHNIQUES

UNIT – I

[16 HOURS]

Fundamentals of chromatography: General description, definition, terms and parameters used in chromatography, classification of chromatographic methods, criteria for selection of stationary and mobile phase-nature of adsorbents, factors influencing the adsorbents, nature and types of mobile phases and stationary phases.

Column chromatography: Theories – plate theory, rate theory, band broadening-eddy diffusion, longitudinal diffusion and resistance to mass transfer, column efficiency, Van Deemter’s equation and its modern version, optimization column performance, interrelationships-capacity factor, selectivity factor, column resolution, distribution constant and applications of conventional column chromatography, advantages and limitations.

Thin layer chromatography (TLC): Definition, mechanism, efficiency of TLC plates, methodology –selection of stationary and mobile phases, preparation of micro and macro plates, development, spray reagents, identification and detection, reproducibility of R_f values, qualitative and quantitative analysis.

Paper chromatography (PC): Definitions, theory and principle, techniques; one, two-dimensional and circular PC, mechanism of separation, types of paper, methodology-preparation of sample, choice of solvents, location of spots and measurement of R_f value, factors affecting R_f values, advantages and applications

High performance liquid chromatography (HPLC)*:* Instrumentation, pumps, column packing, characteristics of liquid chromatographic detectors-UV, IR, refractometer and fluorescence detectors, advantages and applications.

UNIT – II

[16 HOURS]

Gas chromatography (GC): Principle, instrumentation, columns, study of detectors –thermal conductivity, flame ionization, electron capture and mass spectrometry, factors affecting separation, retention volume, retention time, applications.

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

Solvent extraction*:* definition, types, principle and efficiency of extraction, sequence of extraction process, factors affecting extraction-pH and oxidation state, masking and salting out agents, techniques-batch and continuous extraction, applications.

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

References

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

ANALYTICAL CHEMISTRY PRACTICALS – II

[64 HOURS]

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 calcium in calcium gluconate/calcium carbonate tablets/injections and of calcium in milk powder by EDTA titration.
5. Analysis of commercial hypochlorite and peroxide solution by iodometric titration.
6. Determination of ascorbic acid in vitamin C tablets by titrations with $KBrO_3$ and of vitamin C in citrus fruit juice by iodimetric titration.
7. Determination of iron in pharmaceuticals by visual and potentiometric titration using cerium(IV) sulphate.
8. Determination of total cation concentration of tap water by ion-exchange chromatography.
9. Determination of magnesium in milk of magnesium tablets by ion-exchange chromatography.
10. Cation exchange chromatographic separation of cadmium and zinc and their estimation by EDTA titration.
11. Gas chromatographic determination of ethanol in beverages.
12. Determination of aspirin, phenacetin and caffeine in a mixture by HPLC.
13. Anion exchange chromatographic separation of zinc and magnesium followed by EDTA titration of the metals.
14. Separation and determination of chloride and bromide on an anion exchanger.
15. 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 SCT 2.52: INDUSTRIAL INORGANIC CHEMISTRY

[16 HOURS]

UNIT – I

Metal Carbides: salt like, covalent and industrial carbides. Intercalation compounds of graphite, alkali metals. Industrially important recactions of oxides with carbon.
Silicone polymers: Introduction, nature of chemical bonds containing silicon, general methods of preparation (fluids and resins) and properties of silicones. Applications. Industrial uses of silicon, silicon carbide and silicon dioxide.
Chemical reactivity and group trends of germanium, tin and lead: Applications, metallic tin and alloys, lead alloys and oxides of lead.
Compounds of arsenic, antimony and bismuth: Intermetallic compounds and alloys and their uses.
Ceramics: Raw materials used in ceramics and ceramic insulators.

UNIT – II

[16 HOURS]

Inorganic fibers: Introduction, properties, classification, asbestos fibers, optical fibers, carbon fibers, Applications.
Zeolites: Introduction, types of zeolites, manufacture of synthetic zeolites and applications.
Mineral fertilizers: **Phosphorous containing fertilizers** - Economic importance, importance of superphosphate, ammonium phosphates and their synthesis.
Nitrogen containing fertilizers - Importance and synthesis of ammonium sulfate, ammonium nitrate and urea.
Potassium containing fertilizers - Economic importance and manufacture of potassium sulfate.
Inorganic pigments: General information and economic importance.
White pigments – titanium dioxide pigments, zinc oxide pigments.
Colored pigments – Iron oxide, chromium oxide, mixed-metal oxide pigments and ceramic colorants.
Corrosion protection pigments, luster pigments, luminescent pigments, magnetic pigments.

References

1. Inorganic Chemistry Principles of Structure and Reactivity: James E. Huheey, Ellen A. Keiter, Richard L. Keiter, Okhil K. Medhi, Delhi University, New Delhi (2006).
2. Chemistry of the Elements – N.N. Greenwood and A. Earnshaw, Pergamon Press (1985).
3. Industrial Inorganic Chemistry – 2nd edition. K.H. Buchel, H.H. Moretto and P. Woditsh, Wiley - VCH (2000).

CHO SCT 2.53: DYES & INSECTICIDES

UNIT – I

[16 HOURS]

Dyes: Introduction, modern theories of colour and chemical constitution. A general study of the following: Direct azo dyes (congored, rosanthrene O, procion dyes), acid azo dyes (ponceau2R, Naphthol blue black 6B), basic azo dyes (chrysoidin G, bismark brown), developed dyes, mordent dyes, vat dyes, disperse dyes, fibre reactive dyes, sulphur dyes and solvent dyes. Fluoroscent brightening agents (tinopal B.V), cyanine dyes (classification, application in photography, quinoline blue and sensitol), chemistry of colour developer, and instant colour processes.

Synthesis and applications of malachite green, rhodamine-B, phenolphthalein and methyl orange.

Triphenylmethane dyes: crystal violet, pararosaniline, aurin, chromeviolet.

Application of dyes: i. photography ii. DVD, CD and LCD iii. Biological studies and iv. Electronics.

UNIT – II

[16 HOURS]

Insecticides: Introduction, classification, mode of action and synthesis of chlorinated insecticides (DDT, chlordane, heptachlor and hexachlorocyclohexane), Naturally occurring insecticides-pyrethroids-natural pyrethrins-isolation and structures, synthetic pyrethroids, allethrin, cypermethrin, phenvalerate.

Organophosphorous insecticides: Malathion, parathion, DDVP, diazenon.

Carbamate insecticides: Sevin, carbofluron, aldicab, beygon.

Insect Pheromones: Introduction, classification, use in insect pest control. Synthesis of disparlure, faranol, grandisol, brevicomin and bomykol.

Fungicides: Introduction, Inorganic & organic fungicides, Systemic fungicides-types & examples.

Herbicides: Introduction, study of sulfonyl ureas, heterocyclic sulfonamides, heterocyclic amines, dihydropyrano[2,3-*b*]pyridylimidazolinones,pyrrolopyridylimidazolinones,1,2,4-triazine- 3,5-diones, hydroxyoxazolidinones & hydroxypyrrolidinones, pyridine herbicides &

1,3,4-oxadiazoles. Mechanism of action and toxicities of insecticides, fungicides and herbicides.

References

1. A Text Book of Fertilizers, Ranjan Kumar Basak.
2. Agronomy - Theory & Digest, Bidhan Chandra, Krishi Vishwavidyalaya, Mohanpur.
3. Fundamentals of Agronomy, S.S.Cheema, K.Dhaliwal, T.S. Shota, Punjab Agricultural University.
4. Principles and Practices of Agronomy, Shri.S.S.Singh, Allahabad Agricultural Institute.
5. Fertilizers, Organic Manures & Biofertilizers–A Product Quality Guide for Major & Micronutrients, HLS Tandon, Fertilizer Development and Consultation Organisation, New Delhi.
6. Handbook on Fertilizer Technology, Bham Swaminathan & Manish Goswami, The Fertilizer Association of India, New Delhi.
7. Outlines of Chemical Technology, Charles E. Dryden, Affiliated East-West Press, New Delhi.
8. Synthetic Organic Chemistry, G. R. Chatwal, Himalaya Publishing House.
9. Synthesis and Chemistry of Agrochemicals, Vol I & II, ACS, Wahington.
10. Chemistry of Pesticides, K H Buchel.
11. Advances in Pesticide Formulation Technology, ACS.
12. Chemicals for Crop Protection and Pest Managements, M B Green, G.S. Hartley West, Pergamon.
13. Chemistry of Insecticides and Fungicides, Sree Ramulu, Oxford & IBH, 1985.

CHP SCT: 2.54. NANOMATERIALS, SEMICONDUCTORS AND SUPERCONDUCTORS

[16 HOURS]

Chemistry of Nanomaterials: Introduction, nanoparticles, nanotobes (carbon nanotubes, SWNT and MWNT), nano wires, nano fibers and nano gel. Fullerenes and other bulk balls. Graphine and its applications. Quantum dots.

Synthesis: Chemical vapour deposition (CVD), sol-gel, silica-gel, solvothermal, hydrothermal methods, microwave, electrochemical, laser abalation, biologiocal and bacterial methods. Characterization (X- ray, IR, UV and SEM).

Applications of Nanomaterials : Renewable energy (nano solar cells), coloured glasses (gold and silver ruby glasses), chemical sensors, biosensors, SAM, electrical and electronics (RAM). Chemical and photocatalytic applications. Lithography, drug delivery targeting and medical applications, micro-electrochemical machines (MEMS). Inorganic and organic nano porous gel.

UNIT – II

[16 HOURS]

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

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

Reference

1. Hand Book of Nanotechnology, Bharat Bhushan, Springer Publisher.
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).

OPEN ELECTIVE (FOR NON-CHEMISTRY STUDENTS ONLY)

CH OET: 2.1/3.1- CHEMISTRY

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 molecules. VSEPR model to simple molecules.

Concepts of Acids and Bases: Lux-Flood and solvent system concepts. Hard-soft acids and bases.

Ionic Bond: Properties of ionic substances, structures of crystal lattices (NaCl, CsCl, and ZnS). Lattice energy, Born-Haber cycle, uses of Born-Haber type calculations, Born-Lande equation. Ionic radii, factors affecting the radii of ions, radius ratio effects, covalent character in ionic bonds, hydration energy and solubility of ionic compounds.

UNIT – II

[16 HOURS]

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

Separation techniques:-Solvent extraction, continuous extraction, chromatography (principles of TLC, PC, column, GC, ion exchange chromatography) and electrophoresis

Characterization: Detection of elements, estimation of carbon, hydrogen, halogens, sulphur, nitrogen and phosphourous. Detection of functional groups (hydroxyl, carboxyl, keto, ester, amino, nitro, amide, thiol, ether etc) in the unknown samples. Basic principles for the determination of hydroxyl, carboxyl, keto, ester, amino, nitro groups. Estimation of sugars, aminoacids and proteins.

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

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.

UNIT – III

[16 HOURS]

Spectroscopy: UV-VIS Spectroscopy (outer shell electronic spectroscopy): Quantitative aspects of Absorption -Beer's law. Terminology associated with absorption measurements. Limitation of the law: Real, chemical, instrumental and personal. Theory of molecular absorption. Vibration, rotation, fine structure of electronic spectra. Empirical rules for predicting the wavelength of maximum absorption: Olefins, conjugated dienes, cyclic trienes and polyenes -α, β-unsaturated aldehydes and ketones – benzene

IR spectroscopy: Principles, Hook's law, characteristic group frequencies and skeletal frequencies. Finger print region. Identification of functional groups: Alkenes, alkynes, aromatics, carbonyl compounds (aldehydes and ketones, esters and lactones), halogen compounds, sulphur and phosphorous compounds, amides, lactams, amino acids, and imines.

Factors affecting group frequencies and band shapes, conjugation, resonance and inductance, hydrogen bonding and ring strain, tautomerism, cis-trans isomerism. Applications of IR spectra to co-ordinatation compounds,

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, application of NMR.

CH OET: 2.2/3.2 - GENERAL CHEMISTRY

UNIT – I

[16 HOURS]

Periodic Table. 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 molecules. VSEPR model to simple molecules.

Concepts of Acids and Bases: Lux-Flood and solvent system concepts. Hard-soft acids and bases.

Ionic Bond: Properties of ionic substances, structures of crystal lattices (NaCl, CsCl, and ZnS). Lattice energy, Born-Haber cycle, uses of Born-Haber type calculations, Born-Lande equation. Ionic radii, factors affecting the radii of ions, radius ratio effects, covalent character in ionic bonds, hydration energy and solubility of ionic compounds.

UNIT – II

[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. Variation of free energy with temperature and pressure. **Chemical kinetics**: Rate and order of reaction. Factor affecting the rate of reaction. Order of reaction and its determination. Energy of activation and its determination. Brief account of collision and activated complex theories. **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. Electrode potential and construction of electrochemical cells.

Spectroscopy: Rotation spectra of diatomic molecules (rigid and non-rigid rotator model). Principles of determination of bond length and moment of inertia from rotation spectra. **Infrared spectroscopy:** Vibration of diatomic molecules, vibrational energy curves for simple harmonic oscillator. Theory of IR absorption, types of absorption bands. Number of fundamental vibrations and theoretical group frequencies. Important spectral regions, characterization of functional groups and structure of simple molecules – CO_2, H_2O and CH_3COOH.

UNIT – III

[16 HOURS]

Fundamentals of chromatography: General description, definition, terms and parameters used in chromatography, classification of chromatographic methods, criteria for selection of stationary and mobile phase-nature of adsorbents, factors influencing the adsorbents, nature and types of mobile phases and stationary phases.

Column chromatography: Theories – plate theory, rate theory, band broadening-eddy diffusion, longitudinal diffusion and resistance to mass transfer, column efficiency, Van Deemter's equation and its modern version, optimization column performance, interrelationships-capacity factor, selectivity factor, column resolution, distribution constant and applications of conventional column chromatography, advantages and limitations.

Thin layer chromatography (TLC): Definition, mechanism, efficiency of TLC plates, methodology –selection of stationary and mobile phases, preparation of micro and macro plates, development, spray reagents, identification and detection, reproducibility of Rf values, qualitative and quantitative analysis.

Gas chromatography (GC): Principle, instrumentations, columns, study of detectors – thermal conductivity, flame ionization, electron capture and mass spectrometry, factors affecting separation, retention volume, retention time, applications.

References

1. I. L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
2. Morison and Boyd. Organic chemistry..
3. Introduction to stereochemistry – K. Mislow.
4. R. K. Bansal, Organic Reaction Mechanism, Wiley Eastern Limited, New Delhi, 1993.
5. J. March, Advanced Organic Chemistry, Wiley Interscience, 1994.
6. E. S. Gould, Mechanism and Structure in Organic Chemistry, Halt, Rinhart & Winston, New York, 964.
7. A Guide book to mechanism in Organic Chemistry – Petersykes
8. Stereochemistry and mechanism through solved problems – P. S. Kalsi.
9. F. A. Carey and Sundberg, Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York, 1990.
10. Physical Chemistry by P.W. Atkins, ELBS, 4th edition, Oxford University Press (1990).

11. Text Book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2^{nd} edition (1974).
12. Elements of Physical Chemistry by Lewis and Glasstone.
13. Fundamentals of Molecular Spectroscopy, C.N. Banwell and E.M. McCash. 4^{th} edition, Tata McGraw Hill, New Delhi.

THIRD SEMESTER

CHI HCT: 3.1. ADVANCED INORGANIC CHEMISTRY

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 in organometallics. **Ferrocene and ruthenocene**: Preparation, structure and bonding.

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

UNIT – II

[16 HOURS]

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

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

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

Biological and Medicinal Applications: Organomercury, boron, silicon and aresenic compounds

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

UNIT – III

[16 HOURS]

Chemistry of main group elements: Diborane and its reactions, polyhedral boranes (preparation, properties, structure and bonding). Wade's rules, carboranes and borazines. Inorganic chains, rings and cages of boron, carbon and phosphorous.

Silicates: Structure, classification - silicates with discrete anions, silicates containing chain anion, silicates with layer structure, silicones with three dimensional net work and applications.
Silicone: General methods of preparation, properties. Silicone polymers - silicone fluids, silicone greases, silicone resins, silicone rubbers and their applications.
Heterocyclic inorganic ring system: Sulphur-nitrogen ring, nitrogen-phosphorous ring
Phosphonitrilic or phosphazine polymers: Preparation, properties, structure and 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, Chistoph Elschenbroich 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. Keiter, Richard L. Keiter, Okhil K. Medhi, Delhi University, New Delhi (2006)
9. Chemistry of the Elements – N.N. Greenwood and A. Earnshaw, Pergamon Press (1985).
10. Inorganic Chemistry - 2nd edition, D.F. Shriver, P.W. Atkins and C.H. Langford, Oxford University Press, (1994).

CHO HCT: 3.2. REAGENTS IN ORGANIC SYNTHESIS

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

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. H. Pine, Hendrickson, Cram and Hammond, Organic Chemistry, Mc Graw Hill, New York, 1987.
2. I.L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
3. R.K. Bansal, Organic Reaction Mechanism, Wiley Eastern Limited, New Delhi, 1993.
4. J. March, Advanced Organic Chemistry, Wiley Interscience, 1994.

5. F.A. Carey and Sundberg, Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York, 1990.
6. S.K. Ghosh, Advanced General Organic Chemistry, Book and Alleied (P) Ltd, 1998.
7.

CHP HCT: 3.3. PHYSICAL CHEMISTRY – III

UNIT – I

[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 method.

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. Preparation and properties of colloids. Stability of colloids. Micelles: Surface active agents – micellisation, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants. Micellar catalysis.

UNIT – II

[16 HOURS]

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

Radiation chemistry: Introduction, units, interaction of electromagnetic radiation with matter, G-value, LET of radiation. Chemical dosimetry - Fricke and ceric sulphate dosimeters. Radiolysis - cysteine, 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.

UNIT – III

[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.

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.

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

References

1. Text Book of Polymer Science, F.W. Billmeyer, Jr., John Wiley, London (1994).
2. Polymer Science. V. R. Gowrikar, N.V. Vishwanathan and J. Sreedhar, Wiley Eastern, New Delhi (1990).
3. Fundamentals of Polymer Science and Engineering. A. Kumar and S.K. Gupta, Tata – McGraw Hill New Delhi (1978).
4. Polymer Characterization, D. Campbell and J.R. White, Chapman and Hall, New York.
5. Fundamental Principles of Polymer Materials, R.L. Rosen, John Wiley and Sons, New York.
6. Functional Monomers and Polymers by K. Takemoto, Y. Inaki and P.M. Ottenbrite, Marcel Dekker, Inc., New York, 1987.
7. Physical Chemistry by P.W. Atkins, ELBS, 5th edition, Oxford University Press (1995).
8. Text Book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2nd edition (1974).
9. Nuclear Chemistry by Friedlander and Kennedy, John Wiley and Sons (1987).
10. Essentials of Nuclear Chemistry by H.J. Arnikar, Eastern Wiley (1990).
11. Nuclear Chemistry by U.N. Dash, Sultan Chand and Sons (1991).
12. Fundamentals of Radiochemistry by D.D. Sood, A.V.R. Reddy and N. Ramamoorthy

13. Nuclear Radiation Detectors by S.S. Kapoor and Ramamoorthy, Wiley Eastern (1986).

CHA SCT 3.41: APPLIED ANALYSIS – I

UNIT – I

[16 HOURS]

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

Air quality monitoring: Sampling methods and devices for particulates and gaseous pollutants. SO_2: ambient air measurements and stack gas measurements - Turbidimetric, colorimetric, conductometric and coulometric methods, NOX: Griess-ilosvay and Jacobs-Hockheiser colorimetric methods, chemiluminiscent technique, CO: NDIR, amperometric, FID and catalytic oxidation methods. Hydrocarbons: total and individual hydrocarbons by gas chromatography. Oxidants and ozone: colorimetric, coulometric, titrimetric and chemiluminescence methods.

Air Pollution control: Atmospheric cleaning processes, approaches to contaminant control-detection and control at source.

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

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

UNIT – II

[16 HOURS]

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

References

1. Standard Methods of Chemical Analysis, A.J. Weleher (Part B), Robert E. Kriegor Publishing Co. USA, 1975.
2. Environmental Chemistry, S.E. Manahan Willard grant press, London, 1983.
3. Environmental Chemical Analysis, Iain L Marr and Malcolm S. Cresser, Blackie and Son Ltd., London, 1983.
4. Chemistry for Environmental Engineering, Chair N. Sawyer and Perry L.M Canty, Mcgraw Hill Book, Co., New York, 1975.
5. The Air Pollution Hand Book, Richard Mabey, Penguin, 1978.
6. The Pollution Hand Book, Richard Mabey, Ponguin 1978.
7. Soil Chemical Analysis, M.L. Jackson, Prentice Hall of India Pvt, Ltd., New Delhi, 1973.
8. Experiments in Environmental Chemistry, P.D. Vowler and D.W. Counel, Pergamon press, Oxford 1980.
9. Manual Soil Laboratory Testing, vol I, K.H. Head, Pentech Press, London 1980.
10. A Text Book of Environmental Chemistry and Pollution Control, S.S. Dara, S. Chand and co. Ltd. New Delhi 2004.
11. Air pollution Vol II edition by A.C. Stern, Academic Press New York, 1968.
12. Instrumental Methods for Automatic Air Monitoring Systems in Air Pollution Control, Part-III edition by W. Stranss, John-Wiley and Sons, New York, 1978.
13. Analysis of Air pollutants, P.O. Warner, John Wiley and Sons, New York, 1976.
14. The Chemical Analysis Air pollutants, Interscience, New York, 1960.
15. The Analysis of Air Pollutants, W. Liethe, Ann Arbor Science Pub. Inc. Michigan 1970.
16. Environmental Chemistry, A. K. De.

ANALYTICAL CHEMISTRY PRACTICALS – III

[64 HOURS]

PART – III

1. Determination of calcium in limestone by redox, acid-base and complexation titrations.
2. Determination of vitamin C in orange juice by titration with cerium(IV) and with 2,6-dichlorophenol indophenol.
3. Determination of aluminium and magnesium in antacids by EDTA titration.
4. Determination of saccharin in tablets by precipitation titration.
5. Determination of sulpha drugs by potentiometry using $NaNO_2$ and iodometric assay of penicillin.
6. Determination of iron in mustard seeds and phosphorus in peas by spectrophotometry.
7. Analysis of waste water for anionic detergents and phenol by spectrophotometry.
8. Determination of manganese in steel by extraction-free spectrophotometry and molybdenum in steel by extractive spectrophotometry.

9. Analysis of waste waters for DO and COD by titrimetry.
10. Analysis of a ground water sample for sulphate by titrimetry (EDTA) and turbidimetry.
11. Catalytic determination of traces of selenium in biological materials and iodide in blood serum.
12. Photometric and potentiometric titration of iron(III) with EDTA.
13. Analysis of brackish water for chloride content by a) spectrophotometry (mercuric thiocyanate method), b) conductometry (silver nitrate) and c) potentiometry (silver nitrate).
14. Conductometric titration of sodium acetate with HCl and NH_4Cl with NaOH.
15. Determination of fluoride in drinking water/ground water by spectrophotometry (alizarin red lake method).
16. Analysis of waste water for
    a) phosphate by molybdenum blue method
    b) ammonia-nitrogen by Nessler's method
    c) nitrite-nitrogen by NEDA method
15. Analysis of a soil sample for
    a) calcium carbonate and organic carbon by titrimetry.
    b) calcium and magnesium by EDTA titration.
16. Analysis of a soil sample for
    a) Available phosphorus by spectrophotometry.
    b) Nitrate-nitrogen/nitrite nitrogen/ammonia nitrogen by spectrophotometry.
    c) sodium and potassium by flame photometry.
17. Analysis of urine for
    a) urea and uric acid by titrimetry snd spectrophotometry.
    b) Sulphate by precipitation titration after ion-exchange separation.
    c) Sugar by Benedict's reagent.
18. Analysis of blood for
    a) cholesterol by spectrophotometry
    b) bicarbonate by acid-base titration

References

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.
2. Analytical Chemistry, G.D. Christian, 5th edition, 2001 John Wiley & Sons, Inc. India.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993, prentice Hall, Inc. New Delhi.
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003 Pearson Education Pvt. Ltd., New Delhi.
5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.

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

CHI SCT 3.42: FRONTIERS IN INORGANIC CHEMISTRY

UNIT – I

[16 HOURS]

Materials chemistry

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

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

Chalcogenides, intercalation chemistry and metal rich phases: Layered MS_2 compounds and intercalation, Chevrel phases.

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

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

Molecular materials and 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, nanoscience and nanotechnology

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

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

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

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

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

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

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.

INORGANIC CHEMISTRY PRACTICALS – III

[64 HOURS]

PART – I

1. 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.
2. Flame photometric determination of the following metal ions from different samples:
   a) sodium b) potassium c) calcium d) lithium and d) sodium and potassium in a mixture.
3. Polarographic estimation of cadmium and zinc.

4. Determination of iron as the 8-hydroxyquinolate by solvent extraction method.
5. Quantitative determination of nickel using dithizone and 1,10-phenanthroline by synergistic extraction.
6. Spectrophotometric determination of the *p*Ka value of methyl red.
7. Determination of chromium(III) and iron(III) in a mixture: Kinetic masking method.
8. Semimicrogravimetric estimation of aluminium.

PART – II

9. 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 Tanabe Sugano diagram.
10. Using chloropentamine cobalt(III) chloride, prepare nitro and nitritopentamine cobalt(III) chloride. Record the IR spectra of the isomers and interpret.
11. Estimate the chloride ion in a given complex by silver nitrate titration after ion-exchange separation.
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 hexamine 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. Demonstration Experiments:
    (a) Recording and interpretation of IR and NMR spectra of complexes.
    (b) Spectrochemical series - Evaluation of Dq value.
    (c) DNA interaction with metal complexes by UV-visible absorption and viscosity methods.

References

1. Advanced Physico-Chemical Experiments – J. Rose.
2. Instrumental Analysis Manual - Modern Experiments for Laboratory – G.G. Guilbault and L.G. Hargis.

3. A Text Book of Quantitative Inorganic Analysis – A.I. Vogel, 5th edition.
4. Experimental Inorganic Chemistry – G. Palmer.
5. Inorganic Synthesis – O. Glemser.
6. Experimental Inorganic/Physical Chemistry- Mounir A. Malati.
7. Quantitative Chemical Analysis – Daniel C. Harris, (2006) 7th edition.
8. Spectrophotometric Determination of Elements – Z. Marczenko.

CHO SCT 3.43: CARBOHYDRATES, PROTEINS AND NUCLEIC ACIDS

UNIT – I

[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 – II

[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. L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.

2. K. Albert, L. Lehninger, D.L. Nelson, M.M. Cox, Principles of Biochemistry, CBZ publishers, 1st edition, New Delhi, 1993.
3. Harper's Biochemistry, Ed. R.Harper, 22nd edition, Prentice Hall Press, New York, 1990.

ORGANIC CHEMISTRY PRACTICALS – III

PART – I

[64HOURS]

Isolation of natural products & estimations:

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 azeleic acid from castor oil
6. Estimation of ketones by haloform reaction
7. Estimation of sugars by Bertrand's method
8. Estimation of nitro groups
9. Estimation of amino group
10. Determination of iodine value of an oil or fat
11. Determination of saponification value of an oil
12. Determination of equivalent weight of carboxylic acid by silver salt method

PART – II

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

References

1. Manual of Organic Chemistry - Dey and Seetharaman.
2. A Text Book of Practical Organic Chemistry – A.I. Vogel, Vol. III
3. Practical Organic Chemistry - Mann & Saunders.
4.

CHP SCT: 3.44. APPLICATIONS OF ELECTROCHEMISTRY AND CORROSION

UNIT – I

[16 HOURS]

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

Energetics of cell reactions: Effect of temperature, pressure and concentration on energetics of cell reactions (calculation of ΔG, ΔH and ΔS).

Electrochemical measurements: Amperometry, coulometry at controlled potential and at constant current. Cyclic voltammetry – basic principles, instrumentation and applications.

Electrogravimetry: Theory, electrode reactions, electroplating of metals, electro-deposition of alloys, characteristics of good deposit, completeness of deposition, separation of metals at controlled cathode potential. Determination of copper and nickel in Cu-Ni alloy.

UNIT – II

[16 HOURS]

Corrosion: Manifestations of corrosion, types of corrosion, basis of electrochemical corrosion, theories of corrosion. Local cell theory (Wagner and Traud theory). Current – potential relations (Evan diagram) in corrosion cells. Effect of *p*H, nature of metal and dissolved oxygen (principle of differential aeration) on corrosion. Corrosion rate measurement by different methods – chemical and electrochemical methods (potentiodynamic polarization and AC impendence). General aspects of corrosion prevention and control. General classification of corrosion control methods – designing aspects, effect of allying and surface modification. Corrosion prevention by painting, phosphating and anodic (passivation) and cathodic protection.

Corrosion inhibitors: Introduction, classification – passivating (anodic), cathodic, organic, precipitation and volatile corrosion inhibitors. Green inhibitors and their significance. Corrosion inhibition mechanism, synergism of corrosion inhibitors. Application of potentiodynamic polarization, impendence and IR and UV-visible spectroscopy for the study of behaviour of corrosion inhibitors.

Reference

1. Text Book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2nd edition (1974).
2. Elements of Physical Chemistry by Lewis and Glasstone.
3. Physical Chemistry – G.M. Barrow, McGraw Hill International Service (1988).
4. Introduction to Electrochemistry by S. Glasstone.
5. Electrochemistry –Principles and Applications by E.G. Potter.
6. Electrochemistry by Reiger, Prentice Hall (1987).
7. An introduction to metallic corrosion and its prevention, Raj Narayan, Oxford and IBH Publishing Co. Pvt. Ltd., New Delhi.

8. Fundamentals of metallic corrosion, Philips A. Schweitzer, CRC press Taylor and Francis group, New York.
9. Corrosion: Fundamentals, testing and protection, Thomas A. Adler et al., ASM International.
10. Analytical methods in corrosion science and engineering, Philippe Marcus and Florian Mansfeld, Taylor and Francis group, New York.
11. Corrosion prevention and control, Baldev Raj, U Kamachi Mudali & S. Rangarajan, Narora Publishing House, India.
12. Corrosion Engineering, Fontana & Mars, Tata Mc Graw Hill Education Pvt ltd., India.

PHYSICAL CHEMISTRY PRACTICALS – III

[64 HOURS]

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1. To study the kinetics of saponification of ethyl acetate by conductivity method, determination of the energy of activation.
2. Study of kinetics of reaction between $K_2S_2O_8$ and KI, second order, determination of rate constants at two different temperatures and E_a.
3. Study the salt effects on kinetics of reaction between $K_2S_2O_8$ and KI.
4. Conductometric titration of thorium nitrate with potassium tartarate.
5. Conductometric titration of orthophosphoric acid against NaOH.
6. Conductometric titration of a mixture of HCl, CH_3COOH and $CuSO_4$ against NaOH.
7. Potentiometric titration of mixture of weak acids against NaOH.
8. Conductometric titration of potassium iodide with mercuric perchlorate.
9. To study the acid catalysed kinetics of oxidation of glycine by chloramine-T (CAT) - determination of order of reaction w.r.t. [CAT] and [glycine].
10. Potentiometric titration of $Pb(NO_3)_2$ *vs* EDTA.
11. Potentiometric titration of mixture of KCl+KBr+KI *vs* $AgNO_3$.
12. Study of phase diagram of a three component system (e.g. acetic acid-chloroform water and system).
13. Study of corrosion rate of mild steel in the presence of corrosion inhibitor by mass loss method at different temperature – determination of thermodynamic parameters.
14. Kinetics of decomposition of diacetone alcohol by NaOH - determination of energy of activation and other thermodynamic parameters.
15. Spectrophotometric kinetics of oxidation of indigocarmine by chloramine-T (CAT) – (a) Determination of order of reaction w.r.t. [CAT] (b) Effect of pH and determination of order w.r.t.$[H^+]$.
16. Kinetic study on Ru(III) catalysed reaction between primary amine and CAT (a) Determination of order of reaction w.r.t. [amine] and [CAT] (b) Determination of E_a and thermodynamic parameters.

17. Kinetics of saponification of ethyl acetate by conductivity method and study the effect of dielectric constant of the medium (using CH_3OH).
18. Study of photolysis of uranyl oxalate (a) determination of intensity of light source (b) study of photocatalysis of oxalic acid.
19. Determination of rate of photolysis of CAT/CAB solution.
20. Determination of *p*K value of an indicator (methyl orange).
21. Spectrophotometric analysis of a mixture of (a) $KMnO_4$ and $K_2Cr_2O_7$.
22. Study of complex formation between ferric salt and salicylic acid.
23. Determination of half-wave potential of metal ions in a mixture (Mn^{2+}, Cd^{2+} and Zn^{2+}).
24. Estimation of metal ion in solution by polarographic method.
25. Determination of half-life of ^{40}K using GM counter.
26. Determination of energy gap of a semiconductor by four probe method.
27. Synthesis of nanomaterial (ZnO) by electrochemical method and its application for photodegradation studies.

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.

NON-COMPOSITE

CHI SCT 3.51: BIOINORGANIC PHOTOCHEMISTRY

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 photoprocesses 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; Photobiostimulation, Photoactivation 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

metallopharmaceuticals, 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 detoxifi cation. 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 3.52: LIPIDS, PORPHYRINS, ANTHOCYANINS AND FLAVONOIDS

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 PGE_1. Synthesis of PGE & F series.

Terpenoids: Introduction, classification and general methods of structural elucidation. Biological importance of terpenoids. Chemistry of pinene, camphor, caryophyllene, santonin, abietic acid and vetivone.

UNIT – II

[16 HOURS]

Porphyrins: Introduction, structure and biological functions of haemin. Vitamin $B_{12:}$ 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

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

References

1. L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
2. K. Albert, L. Lehninger, D. L. Nelson, M. M. Cox, Principles of Biochemistry, CBZ publishers, 1st edition, New Delhi, 1993.
3. Harper's Biochemistry, Ed. R.Harper, 22nd edition, Prentice Hall Press, New York, 1990.
4. Encyclopedia of Chemical technology – Kirck-Othmer series.
5. Harper's review of biochemistry – P. W. Martin, P. A. Mayer & V. W. Rodfwell, 5th edition, Maurzen Asian Edition, California, 1981.

CHP SCT: 3.53 APPLICATIONS OF X-RAY CRYSTALLOGRAPHY AND QUANTUM CHEMISTRY

UNIT –I

[16 HOURS]

Applications of X-ray crystallography: Crystal growth techniques. Data collection, Data reduction, Structure solving and refinement, Shelx-2013, Olex-2, WinGX, Encifer, PLATON, MERCURY, SUPERFLIP, ORTEP, Packing, R-value, CIF, CIF-Tab, Disorder, polymorphism & pseudopolymorphism, Hydrogen bonding interactions, Bifurcated and trifurcated hydrogen bonding.

UNIT –II

[16 HOURS]

Applications of quantum mechanics: Application of variation theorem to a particle in one dimensional box, linear oscillator, H and He-atoms, 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-Slater's orbitals for He, Carbon and nitrogen. Theories of valence – Introduction, linear and non-linear variation functions, secular equations, coulombic, exchange, normalization and overlap integrals, secular determinants.

References

1. Structure determination by x-ray crystallography by Mark Ladd & Rex Palmer
2. An Introduction to X-ray crystallography by M. M. Woolfson
3. Crystal Structure Determination by Werner Massa & Robert O. Gould
4. Crystal Structure Determination (Oxford Chemistry Primers) by William Clegg
5. X-Ray Structure Determination: A Practical Guide, 2nd Edition by George H. Stout & Lyle H. Jensen
6. Crystal Structure Refinement: A Crystallographer's Guide to SHELXL (International Union of Crystallography Texts on Crystallography) [Hardcover] by Peter Müller , Regine Herbst-Irmer , Anthony Spek, Thomas Schneider & Michael Sawaya
7. Crystal Structure Analysis:A Primer by Jenny Pickworth Glusker, Kenneth N. Trueblood
8. Crystal Structure Analysis for Chemists and Biologists by Jenny P. Glusker, Mitchell Lewis, Miriam Rossi
9. Crystal structure analysis: principles and practice by Alexander J. Blake, William Clegg, Jacqueline M Cole
10. Principles of X-ray Crystallography by Li-Ling OOi (Oxford Univ Press).
11. A Practical Guide to solving single crystal structures by Manuel A. Fernandes
12. Quantum Chemistry – A.K. Chandra. Second Edition, Tata McGraw Hill Publishing Co. Ltd., (1983).
13. Quantum Chemistry – Eyring, Walter and Kimball. John Wiley and Sons, Inc., New York.
14. Quantum Chemistry –I.N. Levine. Pearson Education, New Delhi, (2000).
15. Theoretical Chemistry – S. Glasstone. East West Press, New Delhi, (1973).
16. Quantum Chemistry – R.K. Prasad, New Age International Publishers, (1996).
17. Valence Theory – Tedder, Murel and Kettle.

18. Quantum Chemistry – D.A. McQuarrie.
19. Theoretical Inorganic Chemistry – Day & Selbin

FOURTH SEMESTER

CHI HCT: 4.1. BIOINORGANIC CHEMISTRY

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. Oxidative phosphorylation and respiratory chain.

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

Biochemistry of calcium: Introduction - comparison of 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 B_{12} and Coenzymes: Structural feature, names of different forms, chemistry of cobalamin, biochemical functions of cobalamins, model compounds. Special characteristics of B_{12} co-enzyme. Photosystems.

UNIT – II

[16 HOURS]

Metal ion transport and storage: Iron storage and transport: Transferrin, ferratin, phosvitin and gastroferrin. Iron transport in microbes: siderophores, *in vivo* microbial transport of iron

Oxygen transport and oxygen uptake proteins: Properties of dioxygen (O_2): Thermodynamic and kinetic aspects of dioxygen as an oxidant, activation of dioxygen through complexation with metal ions.

Haemoglobin (Hb) and Myoglobin (Mb) in oxygen transport mechanism: Introduction to porphyrin system, substituent effects on porphyrin rings, functions of Hb and Mb. Characteristics of O_2^- binding interaction with Hb and Mb. Model compounds for oxygen carriers (Vaska's complex and cobalt(III) – Schiff base complexes). Hemerythrin and hemocyanin.

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

Superoxide dismutase: Structure and reactivity.

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

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

UNIT – III

[16 HOURS]

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

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

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

Treatment of toxicity due to inorganics: General aspects of mechanism of metal ion toxicity,

(i) Mechanism of antidote complex with poison, rendering it inert: arsenic, lead, mercury, iron, copper

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

References

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

CHO HCT: 4.2. PHOTOCHEMISTRY, PERICYCLIC REACTIONS AND ORGANOMETALLIC CHEMISTRY

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), organomanganese, 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. Organosamarium reagents: Reactions promoted by samarium diiodide and dicyclopentadienyl samarium – Barbier type reaction, Reformatsky type reactions, ketyl- alkene coupling reactions, pinacolic coupling reactions, acyl anion reactions. 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.

i. **Topocity - Prochirality**- Substrate selectivity - Diastereoselectivity and enantio-selectivity-Substrate controlled methods-use of chiral substrates - examples
ii. 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, IPC_2BH, (*S*)-BINAP-DIAMINE and (*R*)-BINAL-H. Use of (*R*,*R*)-DIPAMP, (*S*,*S*)-CHIRAPHOS, (*R*,*R*)-DIOP, SAMP, RAMP, *S*-Proline, *S*-PBMgCl, (-)-$BOAlCl_2$, (+) and (-)-DET.

References

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

CHP HCT: 4.3. PHYSICAL CHEMISTRY – IV

UNIT – I

[16 HOURS]

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

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.

Surface reactions: Langmuir unimolecular and bimolecular reactions.

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]

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.

Statistical thermodynamics: Micro and macro states, phase and ensembles. Thermodynamic probability and most probable distribution – Maxwell-Boltzmann distribution law. Maxwell-Boltzmann, statistics and applications, Bose-Eistein and Feimi-Dirac Statistics. Partition functions – definition, evaluation of translational, rotational and vibrational and electronic for monoatomic, diatomic and polyatomic gaseous molecules. Calculation of thermodynamic functions and equilibrium constants in terms of partition functions, entropy of monoatomic gases. Sackur-Tetrode equation. Comparison of third law and statistical entropies.

UNIT – III

[16 HOURS]

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

Fundamentals of X-ray crystallography: law of interfacial angles, laws of symmetry, Miller indices, Bragg equation, 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.

References

1. Chemical Kinetics by K.J. Laidler.
2. Chemical Kinetics by Frost and Pearson.
3. Kinetics and Mechanism of Chemical Transformation by J. Rajaram and J.C. Kuriacose.
4. Chemical Kinetics by L.K. Jain.
5. Chemical Kinetics by Benson.
6. Text Book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2nd edition (1974).
7. Elements of Physical Chemistry by Lewis and Glasstone.
8. Phase Rule, Gurthu and Gurthu.
9. Statistical Themodynamics by B.C. Meclelland, Chapman and Hall, London (1973).
10. Elementary Statistical Thermodynamics by N.D. Smith, Plenum Press, NY (1982).
11. Elements of Classical and Statistical Thermodynamics by L.K. Nash, Addison-Wesley (1970).
12. Statistical Thermodynamics by I.M. Klotz.
13. Introduction to Statistical Thermodynamics by M. Dole, Prantice Hall, (1962).
14. Solid State Chemistry – N.B. Hannay.
15. Introduction to Solids – Azaroff.
16. Solid State Chemistry and its applications – A.R. West.
17. Principles of the Solid State – H.V. Keer.
18. Basic Solid State Chemistry, 2nd edition, Anthony R. West.
19. Solid State Chemistry: An Introduction, 3rd edition, Lesley E. Smart and Elaine A. Moore.
20. Molecular Structure by Wheatley
21. Physical Chemistry by Barrow
22. Physical Chemistry by Glasstone & Lewis