

FACULTY OF SCIENCE & TECHNOLOGY DEPARTMENT OF CHEMISTRY

for

M.Sc. degree in CHEMISTRY

REGULATIONS & SCHEME OF EXAMINATION

As per CBCS system

With effect from Academic Year 2024-25 [Approved in the BOS meeting held on 26-09-2024]

Submitted by Prof. Basavaraj Padmashali Chairman, Department of Chemistry & BoS in Chemistry, RCUB.

DEPARTMENT OF CHEMISTRY [FACULTY OF SCIENCE & TECHNOLOGY]

Regulations & Scheme of Examination for M.Sc. Degree in Chemistry

1.0 Title of the Course

The course shall be called **M.Sc. in CHEMISTRY**.

1.1 Duration of the course: The M.Sc. degree course is of two years duration, spread over four semesters each of four months duration.

1.2 Eligibility for Admission: The Bachelor's degree in Science or equivalent degree with Chemistry as one of the subject. The candidate should have obtained at least 40% of marks in optional subjects as well as in aggregate. Relaxation in respect of SC/ST/Cat -I etc. will be followed as per prevailing rules of the university.

1.3. Admission & Seat Matrix: The rules for admission & Seat matrix are as per university notification from time to time.

1.4. Admission to other semesters: students are allowed to take admissions to successive semesters under carry over benefit (COB) facility.

- **2.0 Attendance:** Every student must have at least 75% attendance in each paper (Theory & Practical) in each semester. Shortage of attendance will be dealt with as per the university rules from time to time.
 - **3.0** Medium of instruction: The medium of instruction shall be English.

4.0 Course Structure:

There shall be Three category of Papers namely, Core subject (Theory & Practicals), Soft core (50 marks spectroscopy paper), project dissertation and Open Elective (Theory) Papers for M.Sc. in Chemistry.

In the 1^{st} semester, there shall be 4 core theory papers of 4 credits in each paper and 3 core subject practical papers of 2 credits each and 1 soft core paper of 2 credits.

In 2nd semester, there shall be 3 core theory papers of 4 credits in each paper and 3 core subject practicals of each 2 credits, 1 soft core paper of 2 credits and one Open Elective paper with 4 credits.

In 3rd semester, there shall be 3 core theory papers of 4 credits in each paper and 3 core subject practicals each of 2 credits, 1 soft core paper of 2 credits and one Open Elective paper with 4 credits.

In the 4th semester, there shall be 3 core theory papers of 4 credits in each paper and 3 core subjects of <u>practicals each of 2 credits</u>, 1 soft core paper of 2 credits & one **Project** with 4 credits.

Syllabus for Each paper of 4 Credits shall have four Units of 16 h each & Each paper of 2 Credits shall have two Units of 16 h each.

Project work of 4th semester shall be allocated during the 3rd semester itself so that it can be planned well in advance for effective execution under the supervision of Internal and/or External Guide. The Project team shall not exceed *Three* students for a given Topic of study.

5.0 Scheme of Evaluation:

- 5.1 There shall be an examination at the end of each Semester.
- 5.2 The duration of Examination of Theory paper carrying 80 marks is 3 h & duration of Examination of Theory paper carrying 40 marks is 2 h. Duration of Exam for Practicals (Lab) is 4 h and number of students per batch should not exceed 15.

The IA marks of Theory papers are based on average of two IA Tests per Paper per semester as well as Attendance, Seminar and Assignments (if any). The weightage of marks for these components may be distributed accordingly.

The IA marks of Practical paper are based on one IA Tests per Paper per semester.

At least one seminar per Year should be assigned for each student as per the convenience.

- **5.3** The Theory and Practical Examinations of all the semesters shall be evaluated through single / double valuation by an Internal / External examiner as per the guidelines of RCU.
- **5.4 Project:** The project report shall be evaluated for 80 marks by one Internal and one External examiner based on the *Dissertation* & Oral presentation.

IA marks of 20 allocated for Project work must be earned from **Industrial visit/ Technical / Study tour** of minimum 2 days to be undertaken during

the 2nd Yr M.Sc. course. Such a visit/ tour (within India) must be endorsed by the Chairman, Dept. of Chemistry (Principal of Affiliated College). The financial support (partial/full) to the enrolled students and Faculty members accompanying the team may be reimbursed by the University/ Affiliated College, as per the norms.

In case the student cannot undertake **Industrial visit/ Technical / Study tour** due to health issues or unavoidable circumstances, IA marks shall be based on the presentation of the work in a seminar.

6.0 Pattern of question paper: 80 (Exam) + 20 (IA)

Question paper contains five questions. Question 1 is compulsory. It shall contain 10 objective type questions carrying 2 marks each, drawn from all the four units. Questions 2, 3, 4 and 5 should be drawn from each Unit for 16 marks each (sub questions a, b and c or d carry 5, 5 and 6 marks).

- **7.0 Maximum period for the completion of M.Sc. Degree Programe:** There shall be fully carry over system from First to Fourth semesters. Maximum number of years for a student to complete the degree is as specified by the University from time to time.
- 8.0 The General Regulations Governing Post Graduate Programmes under CBCS and Regulation Governing Post Graduate Programmes in the School of Basic Sciences under CBCS of Rani Channamma University, Belagavi are applicable to this course for all the matters not covered under this.

Course structure of M.Sc. degree in CHEMISTRY

*T-Theory, P-Practical/Project

Subjects	Paper	Instruction hrs/	Duration	Marks			Credits
		week	of Exam, h	IA	Exam	Total	
a) 1 st Semester of the PG Program							
Core	4 T	4 🗆 4 = 16	4 🗆 3	4 🗆 20	4 🗆 80	4 🗆 100	4 🗆 4 = 16
Subject	3 P	3 🗆 4 =12	3 🗆 4	3 🗆 10	3 🗆 40	3 🗆 50	3 🗆 2 = 6
Soft Core	1 T	1 🗆 2 =2	1 🗆 2	1 🗆 10	1 🗆 40	1 🗆 50	$1 \ \Box \ 2 = 2$
			Per	Semester	Total of (Credits	24
b) 2nd& 3rd	Semeste	r					
Core	3 T	3 🗆 4 =12	3 🗆 3	3 🗆 20	3 🗆 80	3 🗆 100	3 🗆 4 = 12
Subject	3 P	3 🗆 4 =12	3 🗆 4	3 🗆 10	3 🗆 40	3 🗆 50	$3 \square 2 = 6$
Soft Core	1 T	1 □ 2 =2	1 🗆 2	1 🗆 10	1 🗆 40	1 🗆 50	$1 \ \Box \ 2 = 2$
OEC	1 T	1 🗆 4 =4	1 🗆 3	1 🗆 20	1 🗆 80	1 🗆 100	$1 \ \Box \ 4 = 4$
Semester Total of Credits						24	
4 th Semester							
Core	3 T	3 🗆 4 = 12	3 🗆 3	3 🗆 20	3 🗆 80	3 🗆 100	3 🗆 4 = 12
Subject	3 P	3 \[] 4 = 12	3 🗆 4	3 🗆 10	3 🗆 40	3 🗆 50	$3 \ \Box \ 2 = 6$
Soft Core	1 T	1 □2=2	1 🗆 2	1 🗆 10	1 🗆 40	1 □ 50	$1 \ \Box \ 2 = 2$
Project	1 Pr	1 x 4 =4	Report Evaluation	1 20	1 🗆 80	1 🗆 100	$1 \ \Box \ 4 = 4$
Semester Total of Credits						24	
Program Grand Total of Credits						96	

T - Theory, P- Practical/ Project, OEC-Open Elective

* For earning IA marks of Project work, please refer to Section 5.4 in the regulation.

Papers details		Teaching	Duration	Marks		Credits	
-		h/ week	of Exam, h	Exam	IA	Total	
1 st somostor							
	CHIT 1.1: Inorganic	I Series					
	Chemistry-I	4	3	80	20	100	4
	CHOT-1.2: Organic		2		20	100	
	Chemistry-I	4	3	80	20	100	4
	CHPT-1.3: Physical	4	2	80	20	100	4
Core	Chemistry-I	4	3	80	20	100	4
Sub	CHES-1.5: Analytical	1	3	80	20	100	4
Sub	Chemistry	4					
	CHIPr -1.6: Inorganic	4	4	40	10	50	2
	Chemistry Practicals-I	•	'	10	10	50	2
	CHOPr-1.7: Organic	4	4	40	10	50	2
	Chemistry Practicals-I		•			00	_
	CHPPr -1.8: Physical	4	4	40	10	50	2
	Chemistry Practicals-I						
Soft	CHGT-1.4: Spectroscopy-I	2	2	40	10	50	2
core		20	20	400	100	(00	24
	Total	30	20	480	120	600	24
	CUIT 2.1 · Inorgania	2 semes	ster	1	I		
	Chamistry II	4	3	80	20	100	4
	CHOT-2.2 · Organic						
	Chemistry- II	4	3	80	20	100	4
	CHPT- 2.3: Physical						
Core Sub	Chemistry-II	4	3	80	20	100	4
	CHIPr-2.6 : Inorganic			10	10	-	
	Chemistry Practicals-II	4	4	40	10	50	2
	CHOPr- 2.7 : Organic	4	4	40	10	50	-
	Chemistry Practicals-II	4					2
	CHPPr- 2.8 : Physical	4	4	40	10	50	2
	Chemistry Practicals-II					50	2
Soft	CHGT- 2.4: Spectroscopy-II	2	2	40	10	50	2
core		-	-			100	-
OEC	CHEG- 2.5: Open elective	4	3	80	20	100	4
Total		30	28	480	120	600	24

Course structure of M.Sc. degree in CHEMISTRY

Papers details		Teaching	Duration	Marks		Credits	
· ·		h/ week	of Exam,	Exam	IA	Total	
			h				
3 rd semester							
	CHIT- 3.1: Inorganic Chemistry-	4	3	80	20	100	4
	CHOT- 3.2: Organic Chemistry-	4	3	80	20	100	4
	III CHDT 2.2: Dhysical Chamiotry	1	2	80	20	100	1
Core	III	4	5	80	20	100	4
Sub	CHIPr- 3.6: Inorganic Chemistry	4	4	40	10	50	2
	Practicals-III				10		
	CHOPr- 3.7 : Organic Chemistry	4	4	40	10	50	2
	Practicals-III	4			10		
	CHPPr -3.8: Physical Chemistry	4	Δ	40	10	50	2
	Practicals-III		т	-10	10	50	2
Soft	CHGT- 3.4: Spectroscopy-III	2	2	40	10	50	2
OEC	CHEG- 3.5: Open elective	4	3	80	20	100	4
	Total	30	28	480	120	600	24
		4 th semes	ter				
	CHIT- 4.1: Inorganic Chemistry-		-		•	100	
	IV	4	3	80	20	100	4
	CHOT- 4.2: Organic Chemistry- IV	4	3	80	20	100	4
Core	CHPT- 4.3: Physical Chemistry- IV	4	3	80	20	100	4
Sub	CHIPr -4.6: Inorganic Chemistry	4	4	40	10	50	2
	Practicals-IV		Т	40	10	50	<u> </u>
	CHOPr -4.7: Organic Chemistry	4	4	40	10	50	2
	Practicals-IV			-	_		
	CHPPr 4.8: Physical Chemistry	4	4	40	10	50	2
Coff	Practicals-IV						
core	CHGT- 4.4: Spectroscopy-IV	2	2	40	10	50	2
			Open-				
Proje	CHGP 4.5: Project /Dissertation	4	Report	80	20	100	4
ct			evaluatio				
			n				
	Total	34	28	480	120	600	24
	Grand Total	120	112	1920	480	2400	96

Details of Course structure of M.Sc. degree in CHEMISTRY

 $T: Theory, \ Pr: Practical, P: Project, \ EG: Elective \ General, \ ES: Elective \ Special$

Syllabus of M.Sc. degree in CHEMISTRY

FIRST SEMESTER

CHIT-1.1 : INORGANIC CHEMISTRY-I

Teaching: 4 h/ week & Credits : 4

UNIT-I CHEMICAL BONDING Ionic Bonding

Formation, conditions for the formation of ionic compounds, lattice energy, Born-Lande's equation, calculation of lattice energy from Born-Lande's equation (problems should be solved), conclusions from Born-Lande equation, Born-Haber cycle and its applications (problems should be solved), Kapustinskii equation, factors affecting the lattice energy, properties of ionic substances, Covalent character in predominantly ionic bonds, polarizing power, factors governing the degree of polarization, Fajan's rules in predicting the melting and boiling points and solubility of some compounds.

Energetics of solubility of ionic salts in polar solvents, solvation energy, relative effects of ionic radii on lattice energy and ion-solvation energy, relative solubility of ionic compounds (alkali metal halides and silver halides, sulphates and hydroxides of alkaline earth metals).

Covalent bonding:

Valence bond theory: hybridization of atomic orbitals, Examples for compound having different hybridization (*sp*, *sp*², *sp*³, *dsp*², *sp*³d, *sp*⁻³d²).

VSEPR theory: Predicting molecular geometries, Bent's rule of hybridization, illustration of Bent's rule with respect to CH3F, PCl3F2), limitations of VSEPR theory.

Molecular orbital theory: Symmetry and overlap, molecular orbital diagrams of diatomic homo nuclear molecules/ions (up to second period elements), hetero- nuclear molecules/ions (HCl, LiF, CO, NO, NO⁺ and triatomic molecules–linear (CO2) and angular (NO2). Magnetic properties of the molecules/ions based on the MOT, stability of molecules or ions based on bond order. Walsh diagrams for XH2 species.

Metallic bonding: Characteristics of metallic states, electron sea model, V. B. approach, band theory (MOT).

16 h

Total: 64 h

Self study: Review of different types of chemical bonds with suitable examples. <u>Skill</u> <u>component</u>: Determine the bond energy and calculate the lattice energies and discuss their application.

UNIT-II

CHEMISTRY OF NON-TRANSITION ELEMENTS-I

Electron deficient compounds: Classification of boranes, nomenclature of boranes.: Synthesis, structure and properties of B2H6, B3H9, B4H10, B5H9, B5H11 and B6H10. Polyhedral skeletal electron pair counting using Wade's rules (*styx* numbers): classification of boron clusters using electron pair count.

Carboranes: Classification, Nomenclature, Synthesis of closocarboranes (C2B10 H12). Structural aspect of closo-C2B10H12.

Metalloborane: Synthesis and structural aspects of [B11H11AlCH3]²⁻, [Fe(CO)3B4H8] and [2-CpCoB4H8].

Metallocarboranes: Synthesis of $[(C_2B_9H_{11})_2F_e]^{2\square}$, $[C_2B_9H_{11}F_eC_p]^-$ and $[C_0(C_2B_9H_{11})_2]^-$, Structure and Bonding in $[C_0(C_2B_9H_{11})_2]^{\square}$

Borazines: Synthesis, reactivity and, structure and bonding.

Electron Rich Compounds: Compounds of Noble gases, Preparation and structure and bonding in Xenon compounds (XeF2, XeF4, XeF6, XeOF4, XeO2F2, XeO3, XeO4) based on VBT and VSEPR.

<u>Self study</u>: Electron deficient compound other than Boran and Lewis acids.

<u>Skill component</u>: Demonstration on the handling of redox sensitive and air/moisture sensitive materials.

UNIT-III

COORDINATION CHEMISTRY AND METAL CLUSTERS

Coordination chemistry: Coordination numbers (1 to 7) and their geometries, geometrical isomerism in square planar and octahedral complexes, optical isomerism in octahedral complexes.

Bonding theories: Review of VBT, EAN and their limitations, Spectrochemical series (Irwin-William series), Crystal Field Theory, splitting of d-orbitals in octahedral, tetrahedral, square planar, trigonal bipyramidal and square pyramid geometries, Jahn-Teller distortion in co-ordination compounds. Factors affecting the CFSE values.

Limitations of CFT, evidences for metal ligand orbital overlap, Molecular Orbital Theory with sigma (\Box) bonding applied to octahedral, tetrahedral and square plannar complexes. MO-Theory with $\pi(pi)$ -bonding applied to octahedral complexes.

Metal Clusters

Dinuclear compounds:Quadrapole bonding, calculation of M-M bond order and structural aspects and magnetic properties of Re₂Cl₈².

Trinuclear clusters: Bond order, magnetic properties and structural aspects of Re3Cl9.

<u>Self study</u>: Basics of Coordination Chemistry (Review of VBT, EAN and their limitations).

Skill component: Methods to Identify cis- & trans- as well as L- & D-isomerism.

UNIT–IV 16 h Pi (π) ACID METAL COMPLEXES AND ACID-BASE CHEMISTRY

Metal Carbonyls: Different binding modes of CO, pi (π) acidity of CO, back bonding, synergic effect, mononuclear carbonyls, low nuclearity carbonyl clusters and high nuclearity carbonyl clusters, application of 18 electron rule to metal carbonyls.

Structural features of [Co2(CO)8], [Co4(CO)12] and [Fe3(CO)12].

Preparation and structural aspects of Ni(CO)4, Fe(CO)5 and Co2(CO)8 by direct reaction of metals, V(CO)6, and Mn2(CO)10 by reductive carbonylation.

Metal Nitrosyls: Coordinating behavior of NO, NO as a bridging ligand, factors favoring linear and bent M-N-O linkage, synthesis of nirosyl complexes (brown ring complex).

Dinitrogen Complexes: Reason for poor coordinating behavior of N2 compared to its isoelectronic species, binding modes of N2, preparation of Ru and Mo dinitrogen complexes.

Acid-Base Chemistry: Bronsted-Lowry concept, Lux-Flood theory, solvent-system definition, Lewis theory, Usanovich concept, Hammett acidity function (superacids), HSAB theory.

Self study: structural features of Ni(CO)4, Fe(CO)5 and Co2(CO)8

Skill component: Preparation of one metal nitogen compound and its characterization.

- 01. Inorganic Chemistry: Principles, structure and reactivity, 1997, J. E. Huheey, Keiter and Keiter.
- 02. Inorganic Chemistry, 3rd edition, C. E. Housecroft and A. G. Sharpe.
- 03. Inorganic Chemistry by Purcel and Kotz.
- 04. Inorganic Chemistry by J. D. Lee.
- 05. Inorganic Chemistry by W. W. Porterfield.
- 06. Concepts and Models of Inorganic chemistry by Douglass, Alexander and Mcdaniel.
- 07. Advanced Inorganic Chemistry by Cotton and Wilkinson.
- 08. Inorganic Chemistry by Miessler and Tarr.
- 09. Fundamental concepts of Inorganic Chemistry by A. K. Das, volume 1 to 7.
- 10. Chemistry of Elements by N N Greenwood and A. Earnshaw (2nd Ed) 1997

CHIPr -1.6 INORGANIC CHEMISTRY PRACTICALS-I

Duration: 4 h/ week & Total: 64 h Credits : 2

Part A. Ore Analysis:

- 01. Haematite: Iron by volumetric (potassium dichromate and Ceric ammonium sulphate) method and by colorimetric method
- 02. Pyrolusite: Determination of manganese dioxide in pyrolusite using permanganate titration
- 03. Estimation of calcium and magnesium carbonates in dolomite using EDTA titration, and gravimetric analysis of insoluble residue.

Part B. Alloy Analysis :

- 04. Quantitative analysis of Copper-Nickel in alloy /mixture:
- 05. Copper volumetrically using KIO3.
- 06. Nickel gravimetrically using DMG
- 07. Quantitative analysis of Copper-Zinc in alloy/mixture:
 - i. Copper gravimetrically as Cu(I) thiocyanate.
 - ii. Zinc by volumetrically by EDTA method
- **Part C.** Determination of COD and BOD of polluted water.

Teaching: 4 h/ week & Credits : 4

UNIT-I BASIC CONCEPTS AND REACTION MECHANISM

Concept of hybridization: sp^3 , sp^2 , sp – with examples.

Electronic effects: Inductive, electronic, resonance and hyperconjugation.

Classification of organic reagents and reactions.

Reactive Intermediates: carbocations, carbanions, free radicals, carbenes, nitrenes, and arynes- their formation, stability, structure and reactions.

Organic acid and bases: Effect of substituents with examples

Reaction Mechanism: Classification, determination of reaction mechanism by kinetic and non-kinetic-methods.

Kinetic Method:Mechanistic implications from rate laws, the transition state theory, ambiguities ininterpreting kinetic data, solvent effect, ionic effect, isotopic effect, solvent isotopic effect, substituent effect, steric effect, linear free energy relationships–Hammett equation and Taft treatment.

Non-kinetic methods:Energy profile diagram, identification of products, testing possible intermediates, trapping of intermediates, cross over experiments, isotopic labeling, stereochemical studies, limitations.

<u>Self study (SS)</u>: Basic of atom, molecules, hybridization, ionization energy, electron affinity, electronegativity, delocalization, Bohr theory, Aufbau principle, steric effect, rate of reaction, activation energy, isotopes, stereochemistry.

<u>Skill components:</u> Free radical- ESR spectra of some of the molecule analysed. Carbocation- isolated compound list and analysis.

UNIT-II

ADDITION AND ELIMINATION REACTIONS

Addition reactions: Types of addition reactions, mechanism and stereochemistry of addition, effect of substrates and solvents during addition. Addition to Carbon- Carbon double bond-addition of hydrogen halide(Markonikov's rule), bromine. Addition to carbon-hetero multiple bonds (C=O)-Introduction, structure and reactivity, HCN, bisulphate, Grignard reagent, hydride, amino compounds, alcohols and thiols.

Elimination reactions: Introduction, types of elimination-E1, E2, E1CB mechanisms, orientation during elimination reactions-Saytzeff and Hoffmann rules, pyrolytic eliminations, Chugave, Cope eliminations, Hoffmann degradation and dehalogenation of vicinal di halides, substitution v/s elimination with suitable example.

<u>Self study (SS)</u>: Basics of saturated and unsaturated compounds, Markonikov's and anti-Markovnikov's rule, electrophiles and nucleophiles,

16 h

Total: 64 h

geminal and vicinal compounds, difference between addition and elimination reactions.

<u>Skill components</u>: Analyse some addition and elimination product by FT-IR, UV-vis and NMR spectra available from open access/recorded.

UNIT-III

SUBSTITUTION REACTIONS

Aromatic electrophilic substitution reactions: General mechanism of electrophilic substitution in aromatic systems using examples of nitration, halogenations, sulphonation and Friedal Craft alkylation and acylation.

Orientation effect of disubstitution in aromatic systems with suitable examples.

Nucleophilic substitution at saturated carbon: Mechanism of SN1, SN2, SNi reactions–effect of solvent, substrate and leaving group, neighboring group participation, substitution at vinylic and allylic carbon.

Aromatic nucleophilic substitution reactions: Substitution of hydrogen, substitution other than hydrogen, SNAr reactions, SN1, SN2 and benzyne mechanism, Bucherer reaction.

<u>Self study(SC)</u>: Basics of Aromaticity, electrophiles and nucleophiles, electron withdrawing and electron releasing groups and their examples, difference between solute and solvents, vinylic and allylic groups, acids and bases, saturated and unsaturated carbons, stereochemistry (retension & inversion), rate of reaction and activation energy.

<u>Skill components(SC)</u>: SN¹, & SN² products may be analyzed by polarimeter method and record and analyzed nitration and halogenation products using UV-Vis and FT-IR.

CHOT-1.2 : ORGANIC CHEMISTRY-I

UNIT-IV: STEREOCHEMISTRY

Fisher's projection D,L and R,S configurations - relative and absolute configurations, optical isomerism due to asymmetric carbon atoms - optical isomerism in biphenyls, allenes and spirans - optical isomerism of nitrogenous compounds racemisation and resolution - geometrical isomerism and E,Z configurations, properties of geometrical isomers.

Stereochemistry and stereoisomerism. Conformational isomerism and analysis in acyclic and simple cyclic systems - substituted ethane, cyclopentane, cyclohexane and decalins, optical isomerism - optical activity - molecular dissymmetry and chirality - elements of symmetry.

Methods of asymmetric synthesis: using optically active reagents, optically active substrates and optically active catalysts with suitable examples.

Enantio-selective synthesis and diastereo-selective synthesis

<u>Self study(SS)</u>:Basics of stereochemistry, classification, Isomerism, optical activity, chiral compounds, priority order, cis-trans, dextro-levo, oxidizing and reducing agents, plane of polarization.

<u>Skill components(SC)</u>: Students need to create suitable model for R & S configuration by stick & ball method. Dextro & leavo rotation of some samples recorded data analyzed.

REFERENCE BOOKS:

01. Understanding organic reaction mechanisms, A. Jacob, Cambridge Univ. Press, 1997.

16 h

- 02. Introduction to organic chemistry A. Streitweiser, Jr and C. H. Heathcock, Macmillan, 1985.
- 03. Physical and mechanistic organic chemistry, R.A.Y. Jones, 1st Edn. Cambridge Univ. Press, 1979.
- 04. Mechanisms of molecular migrations, Vols I and II, B. S. Thiagarajan, 1st Edn. Pergamon Press, Oxford, 1979.
- 05. P. J. Garratt in Comprehensive organic chemistry, D. Barton and W. D. Ollis, 1st Edn. Pergamon Press, Oxford, 1979.
- 06. Radicals in organic synthesis, B. Giese, Pergamon Press, 1986.
- 07. Stereoelectronic effects in organic chemistry, P. Deslongchamps, 1st Edn. Pergamon Press, 1983.
- 08. Organic photochemistry, J. M. Coxon and B. Halton, 1st Edn, Cambridge Univ. Press, London, 1974.
- 09. Molecular reactions and photochemistry, C. H. Deputy and D. S. Chapman, 1st Edn. Prentice-hall India, New Delhi, 1972.
- 10. Stereochemistry of carbon compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley & Sons, 1994.
- 11. Stereochemistry, Potapov, MIR, Moscow, 1984.
- 12. Stereochemistry, Nasipuri, D, New Age, 1999.
- 13. Advanced organic chemistry, J. March, 4th Edn. John Wiley, 2008.
- 14. Organic Chemistry, R. E. Ireland Prentice-Hall India, New Delhi, 1975.
- 15. Some modern methods of Organic Synthesis, W. Caruthers, Cambridge Uni. Press London, 2nd Edn. 1998.
- 16. Stereochemistry of organic compounds- Principle and applications, D. Nasipuri, 2nd Edn., New Age International Publishers, 2001.

CHOPr-1.7: ORGANIC CHEMISTRY PRACTICAL-I Duration: 4 h/ week & Total: 64 h Credits : 2

TWO STEP PREPARATIONS

- 01. Preparation of acetanilide from aniline
- 02. Preparation of p-bromoacetanilide from acetanilide
- 03. Preparation of hydrolysis of p-bromoacetanilide to p-bromoaniline
- 04. Preparation of p-nitroacetanilide from acetanilide
- 05. Preparation of hydrolysis of p-nitroacetanilide to p-nitroaniline
- 06. Preparation of bezoic acid from benzaldehyde
- 07. Preparation of 2-hydroxynaphthaldehye from 2-naphthol
- 08. Preparation of 2,4,6 tribromo benzene from aniline
- 09. Preparation of phenylazo- β -naphthol
- 10. Preparation of 1-phenyl-3-methyl-pyrazolone

NOTE: Two preparations are to be given for Practical Examinations.

- 01. Vogel's Text Book of Practical Organic Chemistry, Furniss, Hannaford, Smith and Tatchell, ELBS Longmann
- 02. Advanced Practical Organic Chemistry, N.K. Vishnoi, Vikas, Publishing House
- 03. Handbook of Practical Organic Chemistry, Clark
- 04. Practical Organic Chemistry, O.P. Agrawal

CHPT-1.3 : ADVANCED PHYSICAL CHEMISTRY-I **Teaching hours per week: 04 Credits: 04 Total hours: 64**

UNIT-I

CONCEPT OF QUANTUM CHEMISTRY-I

Quantum Chemistry in Historical Perspective and comparative studies of classical and quantum mechanical phenomenon, Failure of classical mechanics. Marsden experiment and Rutherford theory, black body radiation, Wien's Displacement Law, Planck's Law and Stefan-Boltzmann Law Plank quantum theory, term symbols, Photoelectric, Raman and Compton effects. Hydrogen atom spectrum. Bohr Sommerfeld theory. Uncertainty principle. Wave particle duality. Derivation of Bohr's principle of quantization of angular momentum of electron from de-Broglie's relationship (To be derived). Postulates of quantum mechanics, operators, w properties. Hamiltonian operators and their properties, Schrödinger's equation (with respect to space and time time). Physical significance of and characteristics of wave function, eigen function and eigen values (problems), Application of equation to one dimension box. Self-Study:

Skill development: Applications of quantum chemistry and basics of DFT Software.

UNIT-II

BASICS OF THERMODYNAMICS-I

Review of basic principles of thermodynamics (I and II laws of thermodynamics, concept of free energy and entropy, combined form of first and second laws of thermodynamics. Entropy changes during spontaneous process. Helmholtz and Gibbs free energies. Thermodynamic criteria of equilibrium and spontaneity. Variation of free energy with temperature and pressure. Third law of thermodynamics-calculation of absolute entropies. Real gases and fugacity, Variation of fugacity with temperature and pressure. Thermodynamics of dilute solutions: Raoult's law, Henry's law. Ideal and non-ideal solutions: Liquid-liquid solutions, liquid-solid solutions, multicomponent systems and excess thermodynamic properties. Maxwell's relation (to be derived). Thermodynamic equations of equipartition of energy, Classius-Clapeyron equation (to be derived). Vant-Hoff's equation, integrated form of Van't Hoff's equation. (to be derived).

Skill development: Temperature dependent chemical reactions

UNIT-III

UNIT-IV

FUNDAMENTALS OF ELECTROCHEMISTRY -I

Theory of ionic conductance in solutions, ionic atmosphere, relaxation and electrophoretic effects, Metal/Electrolyte interface: OHP and IHP, potential profile across double layer region, potential difference across electrified interface; structure of the double layer: HelmholtzPerrin, Gouy-Chapman, and Stern models., Debye-Huckel theory of strong electrolytes, Debey-Huckel-Onsagar equation(derivation) and Debey-Huckel limiting law(derivation), Onsagar activity co-efficient, mean ionic strength (Debey-Huckel limiting law). Liquid junction potential and its determination.

Electrical double layer and its structure Helmoltz-Perrin, Guoy-Chapman and Stern models. sedimentation potential, Dorn effect, streaming potential, Zeta potential and its determination, kinetics of electrode process, Butler Volmer equation, Tafel equation, generation of hydrogen. Bio-electrochemistry, biosensors, communication in biological systems.

Skill development: Cyclic Voltammetric Study of ferrocyanide/ferricyanide Redox couple

16 hours

16 hours

16 hours

16 hours

ATOMIC STRUCTURE AND ATOMIC SPECTRA: A brief history of atomic models drawbacks, Bohr theory of Hydrogen atom, Sommerfeld's relativistic atomic model, A wave mechanical concept of the atom. Characteristics of Quantum numbers, Vector atomic model. Brief explanation of doublet structure of alkali spectra (Li, Na and K) and compound doublets, Helium and alkaline earth spectra (Magnesium and Calcium), spark spectra and arc spectra. Moseley lines. Multiplet structure of line spectra, prohibition of inter combinations. Multiplicities and term symbols. Space quantization: Zeeman effect, normal and anomalous Zeeman effects, Paschen- Backeffect, Stark effect.

Skill development: Experimental studies of UV-Vis spectrophotometry

REFERENCE BOOKS:

- 01. Physical chemistry Moore, Orient Longman, 1972.
- 02. Principle of polymer science, by Bhahadur and N.V Shastry, 2nd addition Nonasa, 2011
- 03. An introduction to Chemical Thermodynamics –R. P.Rastogi and S.S.Misra, Vikash, Delhi, 1978.
- 04. Thermodynamics Rajaram and Kunakose, East West, Nagin Cx, Dehli, 1986.
- 05. An introduction to Electrochemistry –Glastone,East west Ltd.
- 06. Electrochemistry principles and applications –Porter
- 07. Introduction to electrochemistry by S. Glasstone.
- 08. Modern electrochemistry Vol. I and II, by J.O.M. Bockris and A.K.N. Reddy, Pentium Press, New York (1970).
- 09. Electrochemistry Principles and applications by E.G. Potter.
- 10. Electrochemistry by Reiger, Prentice Hall (1987).
- Industrial Electrochemistry D. Pletcher and F. C. Walsh, Chapman ,II Edition,1984
- 12. Introductory Quantum Mechanics Atkins ,Claredon,Oxford
- 13. Quantum chemistry-Kauzman, Academic Press, 1957.
- 14. Quantum chemistry-R.K.Prasad ,II.Ed,New Age Int-2000
- 15. Textbook of polymer science –Billmeyer, Willey Intersection.
- 16. Polymer Science- V. R. Gowariker, 2010.

PRACTICALS

- 1. Conductometry
- 2. Acid mixture versus NaOH
- 3. Weak acid with salt versus NaOH
- 4. Strong acid with salt versus NaOH
- 5. To determine the acidic and basic dissociation constant of an amino acid and determination of isoelectric point by pH metry.
- 6. Determine the equivalent conductance at infinite dilution for acetic acid by applying Kohlrausch's law of independent migration of ions.
- 7. Potentiometry
- 8. $K_2Cr_2O_7$ versus FAS
- 9. Acid mixture versus NaOH
- 10. KMnO₄ versus FAS
- 11. Determination of dissociation constant of H₃PO₄ using potentiometric method.
- 12. Determination of pKa value of phosphoric acid by pH meter.
- 13. Determination of DO and COD of a waste water sample by titrimetric method.

- 1. Advanced Physico-Chemical Experiments –J. Rose.
- 2. Practical Physical Chemistry –S.R. Palit.

- 3. Experiments in Physical Chemistry Yadav, Geol Publishing House.
- 4. Experiments in Physical Chemistry Palmer.
- 5. Experiments in Chemistry D.V. Jahagirdar, Himalaya Publishing House, Bombay, (1994).
- 6. Experimental Physical Chemistry –Das. R.C. and Behera B, Tata Mc Graw Hill

Soft-core: CHGT-1.4 SPECTROSCOPY-I Teaching: 2 h/ week & Credits : 2

Total: 32 h

UNIT-I

MICROWAVE and RAMAN SPECTROSCOPY

Electromagnetic radiation: Interaction of radiation with matter-absorption, emission, reflection, refraction, transmission, dispersion, polarization, interference and scattering, natural line width and broadening (Doppler effect), Heisenberg uncertainity and intensity of spectral lines, regions of electromagnetic spectrum and their corresponding energies: rotational, vibrational and electronic transitions and their energy levels.

Microwave spectroscopy: Diatomic molecules-**r**igid and non rigid rotatormodel(No derivation), 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(CO2, CH3F and BCl3), moment of inertia expression for linear tri-atomic molecules, experimental techniques-microwave spectrometer, applications- principles of determination of bond length and

moment of inertia from rotational spectra and determination of dipole moments.

Raman spectroscopy: Introduction, Raman and Rayleigh scattering, Stokes and anti-Stokeslines, polarization of Raman lines, depolarization factor, polarizability ellipsoid, theories of Raman spectra-classical and quantum theory, comparison of Raman and IR spectra, rule of mutual exclusion principle, advantages of Raman spectra.

<u>Self study(SS)</u>: Basic of emission, reflection, refraction, transmission, dispersion, polarization, scattering, Doppler effect, Heisenberg uncertainity, diatomic molecules, isotopes, polyatomic molecules, moment of inertia, tri-atomic molecules, bond length anddipole moments. Basic of Raman Theory, polarisability

Skill component (SC): Raman spectral studies of any two compounds.

UNIT-II

16 h

UV-VISIBLE and INFRARED SPECTROSCOPY

UV-Visible spectroscopy: Modes of electronic excitations and their theoretical interpretation, Beer's law, Lambert's law, Beer's-Lambert's law, limitations, chromophores, auxochromes, effect of substituents on the position of λ max, prediction of λ max for Dienes, α , β -unsaturated aldehydes and ketones (Woodward-Fisher rules), applications of UV-Vis.

FT-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, amides, amino acids, and imines. Factors affecting group frequencies and band shapes, conjugation, resonance and inductance, hydrogen bonding and ring strain, tautomerism, cis-trans isomerism.

<u>Self study(SS)</u>: Basic of IR spectroscopy, Quantum theory of IR, Polarity of bond,.

Skill component (SC): Selected organic compounds recorded/ online source UV-Vis

absorption of benzophenone, benzaldehyde and substituted compounds. And student needs to study, how to calculate molar extinction co-efficient (ϵ), λ_{max} and concentration of some of the molecules/proteins.

Selected organic compounds recorded/collected from online FT-IR and analyzed stretching and bending.

- 01. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash. 4th edition, Tata McGraw-Hill, New Delhi.
- 02. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw-Hill, New York.
- 03. Introduction to Spectroscopy. Pavia, Lampman and Kriz, 3rd edition, Thomson.
- 04. Spectroscopy, B. P. Straughan and S. Walker, John Wiley & Sons Inc., New York, Vol. 1 & 2, 1976.
- 05. Vibration Spectroscopy Theory and Applications, D. N. Satyanarayana, New age International, New Delhi.
- 06. Organic Spectroscopy, William Kemp, 3rd edition, Palgrava, 1991.
- 07. Optical Method of Analysis, E. D. Olsen, McGraw Hill Inc, 1975.
- 08. Spectroscopy of organic compounds P. S. Kalasi, Wiley Eastern Ltd, India 1993.

- 09. Introduction to instrumental analysis R. D. Braun, McGraw Hill Book company 1982.
- 10. Physical methods in inorganic chemistry R. Drago, East West Pvt. Ltd, 1968.
- 11. Instrumental methods of chemical analysis Gurdeep Chatwal and Anand.
- 12. Organic Spectroscopy, 2nd edition– Jag Mohan, Narosa Publishing House New Delhi.
- 13. Applications of IR and Raman spectroscopy to coordination and organometallic compounds, K. Nakamoto.

CHES-1.5: ANALYTICAL CHEMISTRY Teaching: 4 h/ week & Credits : 4

UNIT-I DATA ANALYSIS

Classification of analytical methods: Types of instrumental analysis, analytical methods on the basis of simple size. Errors, types of errors, determinate and indeterminate errors, accuracy and precision. Distribution of random errors, frequency distributions normal error curves. Statistical treatment of finet samples, measure central tendency -mean, medium, range, average deviation, relative average deviation, standard deviation and variance. Students' confidence interval of the mean. Testing for significance, comparison of two means and two standard deviations. Criteria for rejection of an observation-Q test, control chart, propagation of errors, significant figures. Least square methods of deriving calibration of plots. Principles of sampling the sampling step. Methods for sampling solid, liquid and gaseous samples. Effect of sampling uncertainties. Sampling hazards, need for quality assurance: ISO 9000 series of quality of system.

UNIT-II

CHROMATOGRAPHY

Introduction, Principles, classifications, fundamentals of chromatography (Partition coefficient, Retardation factor, retention volumes), Dynamics of chromatography (Efficiency, zone spreading, eddy diffusion), chromatograms, retention time and column efficiency, plate theory and rate theory, Van-Deemeters equation, column resolution, factors influencing resolution.

THIN LAYER CHROMATOGRAPHY

Introduction, stationary and mobile phase systems, Rf value calculation, various technique of developments, visualization and applications.

ION EXCHANGE CHROMATOGRAPHY

Introduction, principle, classification of ion exchange resins, mechanism of ion exchange, synthesis of ion exchange resins (cation and anion), characteristics of ion exchange resins (size, capacity, cross linking and swelling and resistance), and applications.

HIGH PERFORMANCE LIQUID CHROMATOGRAPHY

Introduction, principles, instrumentation, mobile phase, stationary phase, types of column, detectors used, and applications.

<u>Self-study(SS)</u>: Basic of analytical chemistry, types and principle.

<u>Skill components:</u> Prepare TLC plate in laboratory, and run two similar and non-similar aromatic substitution derivatives using suitable mobile phase and calculate Rf values. Collect available online chromatogram for simple organic molecules , and calculate area of the curve and quantification.

16 h

Total: 64 h

masking and salting out agents, techniques-batch and continuous extraction, applications, Separation of lanthanides.

Electrophoresis: Introduction, types and techniques of electrophoresis, factor affecting migration of ions, continuous electrophoresis, thin layer electrophoresis,

moving boundary electrophoresis, zone electrophoresis, and Curtain electrophoresis, reverse osmosis electro dialysis, capillary electrophoresis and applications.

Thermal Methods of Analysis: Introduction, thermogravimetric analysis (TGA), types of thermogravimetric analysis, principle and method, automatic thermogravimetric analysis, instrumentation, types of recording thermobalances, sample holders, factors influencing thermograms and applications, isothermal analysis, Differential Thermal Analysis (DTA), principle of working, theory and instrumentation, simultaneous DTA-TGA curves, factors affecting results and applications. Differential Scanning Colorimetry(DSC), principle of working, theory, instrumentation and applications. Types of titrations and gravimetric analysis.

UNIT-IV

ELECTROANALYTICAL TECHNIQUES

16 h

Introduction, electrochemical cells, faradic and non-faradic current, mass transfer in cells, galvanic and electrolytic cells, anodes and cathodes, liquid junction potential, schematic representation of cells.

Polarography: Theory, principle and applications classical polarography, dropping mercury electrode, polarogram, polarographic measurements, polarographic current, Ilkovic equation, current and concentration relationship, half wave potential, oxygen interference- advantages and limitations. Qualitative and quantitative analysis. Derivative polarography.

Amperometry and Coulometry at controlled potential and at constant current. Cyclic voltametry - basic principles, instrumentation and applications, stripping voltammetry and its applications including Electro -organic synthesis.

Electrogravimetry - theory, electrode reactions, over-voltage, characteristics of a good deposit, completeness of deposition, Determination of copper and nickel in Cu-Ni alloy.

- 01. Principle of Quantitative Chemical Analysis Robert de levie, International edition (1997) McGraw Hill Co.
- 02. Quantitative Analysis- Day and Underwood, Prinitce Hall Indian, Pvt Ltd 6thedition (1993).
- 03. Vogel's Textbook of quantitative chemical analysis- Revised by G.H.jaffery, J. Bassett, J. Mendhm and R.C. Denney ELBS 5thedition (1998).
- 04. Quantitative Chemical Analysis: D.C Harris W.M. Freeman and Co, NY, USA, Ed, (1995).
- 05. Introduction to Instrumental Analysis R.D Brun, McGraw Hill Book company (1982).
- 06. Physical Methods in Inorganic Chemistry- R. Drago, Affiliated to East west Pvt, (1968).
- 07. Introduction to chromatography- theory and practice-V.K. Srivastava and K.K.Srivastava, S. chand Company Ltd., IV Ed (1991).

- 08. Basic Concepts of analytical Chemistry- S.M Khopkar, New Age Intentional Publishers, IIEd.,(1998).
- 09. Analytical chromatography- G.R Chatwal, Himalaya Publishing House, VII Ed., (1998).
- 10. Principle Instrumental Analysis- Skoog, Hollar and Nieman, , Harcourt, Asia pvt Ltd., Indian New Delhi, VEd, (1998).
- 11. Fundamentals of Analytical Chemistry- Skoog, West and Hollar, Harcourt, Asia pvt Ltd., Indian New Delhi, VEd, (1998).

SECOND SEMESTER

CHIT-2.1: INORGANIC CHEMISTRY-II

Teaching: 4 h/ week & Credits : 4

UNIT-I

SYMMETRY AND GROUP THEORY

Molecular symmetry: Symmetry elements and symmetry operations, rotation axis, rules for orientation of molecules, plane of symmetry, rotation-reflection axis, centre of symmetry and identity element of symmetry, products of symmetry operations, general relations among symmetry elements and symmetry operations.

Group theory: Concept of a group, definition of a point group, procedure for classification of molecules into point groups, subgroups, Schoenflies and Hermann-Maugin symbols for point groups, multiplication tables for the symmetry operations of simple molecules, matrix notation for the symmetry elements and for geometric transformations, class of a group and similarity transformation.

Representation of groups: Reducible and irreducible representations, Great Orthogonality theorem and its consequences, labeling of irreducible representations, group theory and hybrid orbitals to form bonds, character tables (Cs, Ci, C2, C2v and C3v).

Applications of group theory: Applications of group theory to crystal field theory, bonding in octahedral and tetrahedral complexes, symmetry and dipole moments, symmetry and optical activity.

<u>Self study</u>: Finding the symmetry elements in compounds with higher CN (> 6) <u>Skill component</u>: Construct the ball and stick model of any chairal compound and deduce the representations.

UNIT-II COORDINATION CHEMISTRY-REACTIONS, KINETICS AND MECHANISMS

Types of mechanisms in substitution reactions-dissociation, interchange and association. Metal-ligand equilibria step-wise and overall stability/formation constant, factors affecting stability of metal complexes. Determination of stability constant by spectrophotometric (Job's) method.

Reactions and kinetics of substitution in square planar complexes: Trans effect, substitution reactions. Rate law and mechanism of nucleophilic substitution in square planar complexes, thermodynamic and kinetic stability.

Reactions and kinetics of substitution in octahedral complexes: Ligand field effects and reaction rates, mechanism of substitution in octahedral complexes, reaction rates influenced by acid and base, mechanism of redox reactions-outer sphere and inner sphere mechanisms. Marcus theory, photochemistry of metal complexes-types of photochemical reactions, photo-substitution and photo-redox reactions and excited

16 h

Total: 64 h

state outer sphere electron transfer reactions (solar energy conversion), complimentary and non-complimentary reactions.

<u>Self study</u>: Fundamental of Solar cell and its reaction mechanism.

<u>Skill component</u>: Find the rate law of substitution reaction using UV-Vis spectrophotometer.

UNIT-III

SOLID STATE AND STRUCTURAL CHEMISTRY

Types of solids, close packing of identical solid spheres, tetrahedral and octahedral voids, packing fraction, radius ratio.

Crystallographic systems: Bravias lattices, Miller indices, external features of crystals. Structures of selected crystals: normal and inverse spinels, hexagonal structures, pervoskites.

Defects in solids: Point defects (stoichiometric and non-stoichiometric), line defects and plane defects, stacking faults and grain boundaries.

Structural transformation of solids

Solid solutions : Hume – Rothery rules, substitutional solid solutions and interstitial solid solutions, solid solution mechanism.

Alloy systems: Phase diagram and their features with respect to alloys - two and three component systems, copper–zinc system, steels with reference to iron-carbon systems.

<u>Self study</u>: X-ray diffraction technique for powder sample and single crystal. <u>Skill</u> component: Indexing of XRD pattern of a cubic system.

UNIT-IV

NUCLEAR CHEMISTRY

Radioactivity, nuclear reactions, nuclear power reactors-radioactivity, determination of half life, radioactive decay kinetics, parent-daughter decay-growth relationships, secular and transient equilibria, nuclear reactions, spallation, nuclear fission and fusion, types of nuclear power reactors, basic features and components of a nuclear power reactor, safety measures, an introduction to breeder reactors, applications of radioisotopes-synthesis of various useful radioisotopes, physico-chemical and analytical applications-isotope dilution method, activation analysis, radiometric titration and ¹⁴C dating, medical, agricultural and industrial applications of isotopes.

RADIATION CHEMISTRY

Interaction of matter with radiation, radiation dosimetry-units and measurement of chemical dosimeters (Fricke and ceric sulphate dosimeters), radiation chemistry of water, a brief introduction to radiolysis of liquids and solids, industrial applications of radiation chemistry (radiation polymerization, food irradiation and radiation synthesis).

16 h

Health and Safety Aspects: Biological effects of radiation, hazards in radiochemical work, radiation protection, decontamination procedures, permissible exposure doses, nuclear waste management including waste storage and disposal procedures.

<u>Self study</u>: Safety measures from radiation field

<u>Skill component</u>: Measuring the radioactivity present in standard sample using GM counter OR construct the Fricke dosimeter and measure the absorbed radiation.

- 01. Symmetry and Spectroscopy of Molecules by K. Veera Reddy.
- 02. Chemical Applications of Group Theory by F. A. Cotton.
- 03. Symmetry and Group theory by P. K. Bhattacharya.
- 04. Inorganic Chemistry: Principles, structure and reactivity, 1997, J. E. Huheey, Keiter and Keiter.
- 05. Inorganic Chemistry, 3rd edition, C. E. Housecroft and A. G. Sharpe.
- 06. Inorganic Chemistry by Purcel and Kotz.
- 07. Inorganic Chemistry by W. W. Porterfield.
- 08. Concepts and Models of Inorganic chemistry by Douglass, Alexander and Mcdaniel.
- 09. Inorganic Chemistry by Miessler and Tarr.
- 10. Introduction to Solids by Azaroff.
- 11. Solid State Chemistry and its Applications by Anthony R. West.
- 12. Solid State Chemistry: An Introduction, 3rd edition, Lesley E. Smart and Elaine A. Moore.
- 13. Fundamental concepts of Inorganic Chemistry by A. K. Das, volume 1 to 7.
- 14. Essentials of Nuclear Chemistry by H.J. Arnikar, Eastern Wiley (1990).
- 15. Nuclear Chemistry by U.N. Dash, Sultan Chand and Sons (1991).
- 16. Nuclear Chemistry by Friedlander and Kennedy, John Wiley and Sons (1987)

CHIPr-2.6: INORGANIC CHEMISTRY PRACTICAL-II Duration: 4 h/ week & Total: 64 h Credits : 2

Part A. Qualitative analysis:

Qualitative analysis of at least FIVE ternary mixtures containing one rare cation and one interfering anion.

Part B. Preparation of complexes:

- 01. K3[Al(C2O4)3] 3H2O & [Cu(thiourea)3]2 SO4. H2O
- 02. Estimation of Copper in tristhiourea copper (I) sulphate by Iodometric method

CHOT-2.2: ORGANIC CHEMISTRY-II

Teaching: 4 h/ week & Credits : 4

Total: 64 h

UNIT-I

NAME REACTIONS

C-C bond forming reactions: Aldol condensation, Reimer-Tiemann reaction, Wittig reaction, Michael addition, Perkin reaction, Corey-Seebach Reaction, Mannich reaction, Shapario reaction. Baylis-Hillman Reaction

C-N bond forming reactions: Stork enamine reaction, Eschweiler-Clarke Reaction, Friedlaender Synthesis, Hofmann-Loffler-Freytag reaction.

C-O bond forming reactions: Sharpless asymmetric epoxidation, Bayer-Villeger reaction.

C-Cl bond forming reaction: Hell-Volhard-Zelinski reaction.

<u>Self-study(SS)</u>: Basic of reaction mechanisms, addition, substitution and rearrangement reactions, and stereochemistry.

<u>Skill components:</u> Aldol condensation, Michel addition & HVZ reaction products were analyzed by various spectroscopic techniques (FT-IR, UV-Vis and NMR spectroscopy) available from online sources.

UNIT-II

OXIDATION AND REDUCTION REACTIONS

Oxidation reactions: Introduction,Oxidation reactions examples and applications of chromium series-K2Cr2O7, PDC, PCC, Sorret and Jones reagents. Manganese compounds-KMnO4, MnO2.

Oxidation reactions involving ozone, peracids, lead tetraacetatate, periodic acid, osmanium tetroxide, selenium dioxide, Oppenauer oxidation.

Reduction reactions: Introduction, Catalytic hydrogenation-both heterogeneous (examples Nickel and palladium) and homogeneous, metal hydride reductions (NaBH4 and LiAlH4), reduction with dissolved metal, diimide reduction, Clemmensen, Wolf Kishner, Meerwin-Varley-Ponndorf reduction, Leukart reaction and reductions with diborane.

<u>Self study(SS)</u>:Basics of oxidation and reduction, calculation of oxidation number, oxidizing and reducing agents with examples.

<u>Skill components(SC)</u>:Oxidizing and reducing agents are identified with model reaction (two examples), and monitor reaction using TLC, UV- Vis and FT-IR.

UNIT –III

REARRANGEMENT REACTIONS

Classification and general mechanistic treatment of nucleophilic, electrophilic and free radical rearrangements.

Rearrangement reactions involving migration to electron deficient carbon: Wolf, Wagner-Meerwein, Pinacol-pinacolone and Benzil-benzilic acid rearrangement.

16 h

16 h

Rearrangement reactions involving migration to electron rich carbon: Favorskii, Sommlet-Houser, Naber and Steven rearrangement.

Rearrangement reactions involving migration to electron deficient nitrogen: Hoffmann, Lossen, Curtius, Schmidt, Beckmann rearrangement.

Rearrangement reactions involving migration to electron deficient oxygen: Dakin, Bayer- Villiger and Hydroperoxide rearrangement.

<u>Self study</u>: Basics of rearrangement, nucleophiles, electrophiles and free radicals with examples, migration and rearrangement of atoms, electron rich and electron deficient atoms.

<u>Skill components(SC)</u>:Students need to give one nucleophilic, electrophilic & free radical rearrangement reactions with suitable examples, analyzereactants and products using spectral data (record/online source).

UNIT-IV

HETEROCYCLIC COMPOUNDS

Nomenclature of heterocyclic compounds-Hantz-Wiedamann system. Synthesis and reactions of

3-Membered heterocyclic compounds – aziridines, azirines, oxiranes, oxirenes and thiiranes.

4-Membered heterocyclic compounds with one and two hetero atoms – azitidines, oxetanes and thietanes

6-Membered heterocyclic compounds with one and two hetero atoms – pyridine, pyrimidine, quinoline.

7-Membered heterocyclic compounds - azepines, oxepines, thiepines.

<u>Self study(SS)</u>: Basics of heterocyclic compounds, nomenclature and examples, aromatic, non-aromatic and anti-aromatic compounds.

Skill components(SC):List out each heterocyclic ring contain drug molecule (one each) and give its biological applications with mechanism/mode of action.

REFERENCE BOOKS:

- 01. Understanding organic reaction mechanisms, A. Jacob, Cambridge Univ. Press, 1997.
- 02. Introduction to organic chemistry A. Streitweiser, Jr and C. H. Heathcock, Macmillan, 1985.
- 03. Physical and mechanistic organic chemistry, R.A.Y. Jones, 1st Edn. Cambridge Univ. Press, 1979.
- 04. Mechanisms of molecular migrations, Vols I and II, B. S. Thiagarajan, 1st Edn. Pergamon Press, Oxford, 1979.
- 05. P. J. Garratt in Comprehensive organic chemistry, D. Barton and W. D. Ollis, 1st Edn. Pergamon Press, Oxford, 1979.
- 06. Radicals in organic synthesis, B. Giese, Pergamon Press, 1986.

- 07. Stereoelectronic effects in organic chemistry, P. Deslongchamps, 1st Edn. Pergamon Press, 1983.
- 08. Organic photochemistry, J. M. Coxon and B. Halton, 1st Edn, Cambridge Univ. Press, London, 1974.
- 09. Molecular reactions and photochemistry, C. H. Deputy and D. S. Chapman, 1st Edn. Prentice-hall India, New Delhi, 1972.
- 10. Stereochemistry of carbon compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley & Sons, 1994.
- 11. Stereochemistry, Potapov, MIR, Moscow, 1984.
- 12. Stereochemistry, Nasipuri, D, New Age, 1999.
- 13. Advanced organic chemistry, J. March, 4th Edn. John Wiley, 2008.
- 14. Organic Chemistry, R. E. Ireland Prentice-Hall India, New Delhi, 1975.
- 15. Some modern methods of Organic Synthesis, W. Caruthers, Cambridge Uni. Press London, 2nd Edn. 1998.
- 16. Stereochemistry of organic compounds- Principle and applications, D. Nasipuri, 2nd Edn., New Age International Publishers, 2001.

CHOPr-2.7: ORGANIC CHEMISTRY PRACTICAL-IIDuration: 4 h/ week & Total: 64 hCredits : 2

PART-A ANALYSIS OF BINARY ORGANIC MIXTURE

Systematic qualitative analysis of binary mixture (solid+solid, solid+ liquid) Chemical equations to be discussed for all tests.

PART-B

Fractional crystallization: Separation of mixture of naphthalene and biphenyl. Fractional distillation: Separation of Mixture of benzene and toluene. Thin layer chromatography: Separation of plant pigments. Column chromatography: Separation of mixture of O & P-nitroanilines.

NOTE: Only experiments in PART-A are to be given in Practical Examination.

REFERENCES

01. Vogel's Text Book of Practical Organic Chemistry	Furniss, Hannaford,
Smith and Tatchell, ELBS Longmann	
02. Advanced Practical Organic Chemistry	N.K. Vishnoi, Vikas,
Publishing House	
03. Handbook of Practical Organic Chemistry	Clark
04. Practical Organic Chemistry	O.P. Agrawal

CHPT-2.3: PHYSICAL CHEMISTRY-II

Teaching: 4 h/ week & Credits : 4

UNIT-I

QUANTUM CHEMISTRY-II

One dimensional simple harmonic oscillator in classical mechanics and quantum mechanics, wave functions of the harmonic oscillators, the applications of Schrödinger's equations to the H atom derivation. Quantization of energy, **Probability distribution function**, normalization of ψ , orthogonality of ψ boundary valued condition, many-electron wavefunctions. Approximate methods in quantum mechanics, variations method, application to the He atom, Slater's determination wave functions, terms symbols and spectroscopic status. Hydrogen like wave functions, angular and radial wave functions and its application to hydrogen atom, application of variation method to hydrogen molecule, ion and normal and degenerate states, Orbital diagram need for variation methods. Perturbation theory, first and second order perturbation theory and its application to linear harmonic oscillator.

Skill development: Brief explanation and experimental results on Density Functional Theory (DFT).

Skill development: Brief explanation and experimental results on Density Functional Theory (DFT).

UNIT-II

STATISTICAL THERMODYNAMICS-II

Statistical thermodynamics: Introduction to statistical thermodynamics, energy states, quantum mechanical and statistical aspects, unit cells, microscopic state and macroscopic state, phase space, system, assembly and ensemble, use of ensemble, microcononical ensemble, canonical ensemble, probability, thermodynamic probability, molecular basis of residual entropy.

Classical statistics, Sterling's approximation, Maxwell Boltzmann distribution law and its applications. Bose-Einstein statistics, Fermi-direc statistics and their comparisons. Derive the relationship between entropy and thermodynamic probability, partition function, thermodynamic functions in terms of partition function (energy, heat capacity, entropy, Gibb's free energy, enthalpy Helmholtz free energy). Evaluation of different types of partition function. i) Translational partition function. Ii) Rotational partition function for diatomic molecule iii) vibrational partition function for diatomic molecule ,electronic partition function iv) nuclear partition function, separation of partition function, residual entropy (problems to be solved).

Skill development: Plotting of radial wave functions using origin software

UNIT-III

CHEMICAL KINETICS: Elementary reactions (Rate law, Order and Molecularity calculations), rate determining step, role of catalyst and Intermediates with examples. Complex reactions: Kinetics of parallel/side, consecutive/sequence, and reversible/opposing reactions. Chain reactions: Branched chain reactions, general rate expression. Theories of reaction rates: Collision theory and its limitations, Activated complex theory (postulates - derivation) and its applications to reactions in solution. Energy of activation, Lindemann theory, Hinshelwood's theory of unimolecular reactions. Potential energy surfaces and **Saddle Point**: Features and construction, theoretical calculations of E_a .

Reactions in solution: Kinetics of salt effects (Primary and secondary salt effect), Cage effect with an example. Fast reactions- Introduction, study of fast reactions by continuous

Total: 64 h

6 h

16 h

and stopped flow techniques, relaxation methods (T-jump and P-jump methods), flash photolysis, pulse and shock tube methods.

Skill development: Kinetics Studies of the Bleaching of Food Dyes

UNIT-IV

PHOTOCHEMICAL REACTIONS

Interaction between light and matter, Importance of Photochemistry, Dark or Thermal reactions, Laws of photochemistry Grottus-Draper law, Stark-Einstein's law of photochemical equivalence, Electronic transitions in molecules, Life times of excited states of atoms and molecules. Jablonski diagram: various processes occurring in the excited state, Non –radiative process (internal conversion, intersystem crossing). Photo physical processes – kinetics of unimolecular reactions, experiments in photochemistry, photo properties –

fluorescence, phosphorescence, chemiluminescence. Delayed fluorescence – E-type and Ptype. State diagrams, Stern-Volmer equation (to be derived), lasers in photochemical kinetic studies. Quantum yield or Quantum efficiency (problems), Experimental Determination of Quantum Yield, Factors affecting the quantum yield. Photosensitized Reactions. Bimolecular processes (Quenching), quantum yields in presence of quenching. Photochemical processes – types of photochemical reactions – electron transfer, photo dissociation, oxidation and isomerization reactions with examples. Photosensitization. Flash photolysis.

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.

Skill development: Degradation of Methylene blue using ZnO or TiO_2 nanosemiconductors.

REFERENCE BOOKS:

- 01. Statistical themodynamics by B.C. Meclelland, Chapman and Hall, London (1973).
- 02. Text book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2 nd edition, (1974).
- 03. Thermodynamics Rajaram and Kunakose, East West, Nagin Cx, Dehli, 1986.
- 04. An introduction to Chemical Thermodynamics–R.P.Rastogi and S.S.Misra, Vikash, Delhi, 1978.
- 05. Introductory Quantum Mechanics Atkins ,Claredon,Oxford
- 06. Quantum chemistry-Kauzman, Academic Press, 1957.
- 07. Quantum chemistry-R.K.Prasad ,II.Ed,New Age Int-2000.

- 08. Physical chemistry-Atkins, ELRS, 1982.
- 09. Physical chemistry –Moore,Orient Longman,1972.
- 10. Quantum Chemistry Eyring, Walter and Kimball. John Wiley and Sons, Inc., New York.
- 11. Theoretical Chemistry S. Glasstone. East West Press, New Delhi, (1973).
- 12. Quantum Chemistry R.K. Prasad, New Age International Publishers (1996).

CHPPr-2.8: PHYSICAL CHEMISTRY PRACTICALS-II

Duration: 4 h/ week & Total: 64 h

Credits : 2

PRACTICAL

Thermodynamics

Solubility: Determine the heat of solution of a solute (e.g oxalic acid or benzoic acid) by solubility method.

Chemical Kinetics

- a. Determine the order and concentration kinetics of the iodination of acetone in the presence of acid by initial rate method.
- b. Study the acid catalyzed inversion of cane sugar and find out: (i) the order with respect to sucrose, (ii)the rate constant, (iii)compare kinetically strength of two acids (HCL and H₂SO₄).
- c. Study of kinetics of autocatalytic reaction between KMnO4 versus oxalic acid.
- **d.** Evaluation of Arrehenius parameter for the reaction between $K_2S_2O_8$ versus KI (first order)

pH metery:

- a. Determination of degree of hydrolysis of aniline hydrochloride at room temperature and calculation of dissociation constant of the base by pH meter.
- b. Determination of pH of acetic acid with sodium acetate buffer by pH meter method.
- c. Determination of pH of formic acid with sodium formate buffer by pH meter method.

Colorimetric:

- a. Determination of dissociation constant of a given indicator by colorimetric method.
- b. Verification of Beers lamberts law by colarimetric method and calculation of molar extinction co-efficient (molar absorption co-efficient)
- c. To construct the calibration curve \overline{Fe}^{2+} -KCNS and Cu^{2+} -NH₃ systems and estimate the amount of respective salt present in a given solution by colarimetrically

- 01. Selected Experiments in Physical Chemistry Latham.
- 02. Experiments in Physical Chemistry James and Prichard.
- 03. Experiments in Physical Chemistry Shoemaker.
- 04. Advanced Physico-Chemical Experiments –J. Rose
- 05. Experimental Inorganic/Physical Chemistry- Mounir A. Malati.
- 06. Quantitative Chemical Analysis Daniel C. Harris, (2006) 7th edition.
- 07. Spectrophotometric determination of elements Z. Marczenko

Soft-core: CHGT-2.4: SPECTROSCOPY-II

Teaching: 2 h/ week & Credits : 2

Total: 32 h

16 h

UNIT-I

NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

Magnetic properties of nuclei (magnetic moment, g factor, nuclear spin), effectof external magnetic field on spinning nuclei, Larmor precessional frequency, resonance conditions, population of nuclear magnetic energy levels, relaxation processes, relaxation time, line width and other factors affecting line width.

Chemical shift, reference standards employed in NMR, factors influencing chemical shift-electronegativity(shielding and deshielding), anisotropic effect, vander Walls deshielding, effect of restricted rotation, H-bonding.

Nature of protons bonded to carbon and other nuclei, Proon integrals, spin-spin couplingcoupling constant, types of coupling, Karplus equations-variation of coupling constants with dihedral angle.

Instrumentation-Frequency sweep instruments, field sweep instruments and pulsed FT-NMR instruments, Chemical equivalence and magnetic equivalence, proton exchange reactions.

First order spectra, non first order spectra, simplification of complex spectra- increasing magneticfield strength, double resonance, deuterium exchange reactions, and lanthanide shift reagents. Nuclear Overhauser Effect (NOE), variable temperature probe.

13C-NMR Spectroscopy: Comparison of ¹H-NMR and ¹³C-NMR, proton decoupling or noise decoupling or broad band decoupling, chemical shift positions of carbon atoms in organic molecules.

Two dimensional NMR Spectroscopy: COSY, NOESY, DEPT Spectra and MRI.

<u>Self study (SS)</u>: Basic of spectroscopy, Electromagnetic radiation, nuclear spin, NMR solvent, theory of NMR.

Skill component (SC): Download NMR spectra of simple molecules: C2H5OH, CH3-

CO-CH3, C6H6, CH3OH and CH3CH2CH2OH, analyse ¹H, ¹³C and 2D NMR data.

UNIT-II

MASS SPECTROMETRY

Introduction, basic theory, instrumentation-single focusing, and double focusing. Methods of generation of positively charged ions-electron impact ionization, chemical ionization, fast atom bombardment (FAB), matrix assisted laser desorption ionization.

Mass analyzer: quadrupole mass filter and TOF.

Resolving power, base peak, molecular ion peak, meta stable peak, isotopic peaks- calculation of percentage intensity of (m+1) and (m+2) peaks. Exact molecular mass, molecular formula, hydrogen deficiency index

Modes of fragmentation-fragmentation rules, McLafferty rearrangement, retro Diels-Alder reaction, ortho-effect, fragmentation of following class of organic compounds – alcohols, aldehydes, ketones, carboxylic acids, and amino compounds.

Combined applications of IR, UV-Visible, ¹H- & ^{f3}C-NMR and mass spectrometry in the structural elucidation of organic compounds. Structure analysis, when spectral data of the organic compound is given

<u>Self study (SS):</u> Origin of mass spectrometry, ionization, principle, types of detector.

<u>Skill component (SC)</u>: Download different functional group containing organic compounds and analyse the fragmentation pattern and justify, how this help for the structure elucidation of new compounds.

REFERENCE BOOKS:

- 01. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash. 4th edition, Tata McGraw-Hill, New Delhi.
- 02. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw-Hill, New York.
- 03. Introduction to Spectroscopy. Pavia, Lampman and Kriz, 3rd edition, Thomson.
- 04. Spectroscopy, B. P. Straughan and S. Walker, John Wiley & Sons Inc., New York, Vol. 1 & 2, 1976.
- 05. Vibration Spectroscopy Theory and Applications, D. N. Satyanarayana, New age International, New Delhi.
- 06. Organic Spectroscopy, William Kemp, 3rd edition, Palgrava, 1991.
- 07. Optical Method of Analysis, E. D. Olsen, McGraw Hill Inc, 1975.
- 08. Spectroscopy of organic compounds P. S. Kalasi, Wiley Eastern Ltd, India 1993.
- 09. Introduction to instrumental analysis R. D. Braun, McGraw Hill Book company 1982.
- 10. Physical methods in inorganic chemistry R. Drago, East West Pvt. Ltd, 1968.
- 11. Instrumental methods of chemical analysis Gurdeep Chatwal and Anand.
- 12. Organic Spectroscopy, 2nd edition– Jag Mohan, Narosa Publishing House New Delhi.
- 13. Applications of IR and Raman spectroscopy to coordination and organometallic compounds, K. Nakamoto.

[OPEN ELECTIVE]

CHEG-2.5: CHEMISTRY FOR EVERY DAY LIFE Teaching: 4 h/ week & Credits : 4 Total: 64 h

UNIT-I POLLUTION

Air pollution: Air pollutants, prevention and control, green house gases and acid rain, ozone hole and CFC's, photochemical smog and PAN, catalytic converters for mobile sources, Bhopal gas tragedy.

Hydrologic cycle, sources, criteria and standards of water quality-safe drinking water, public health significance and measurement of water quality parameters- (colour, turbidity, total solids, acidity, alkalinity, hardness, sulphate, fluoride, phosphate, nitrite, nitrate, BOD and COD), water purification for drinking and industrial purposes.

Toxic chemicals in the environment.

Detergents- pollution aspects, eutrophication. Pesticides and insecticides- pollution aspects, heavy metal pollution, solid pollutants -treatment and disposal, treatment of industrial liquid wastes. Sewage and industrial effluent treatment.

Oils and fats: Composition of edible oils, detection of purity, rancidity of fats and oil, estimation of rancidity, tests for common edible oils Tests for adulterants like aregemone oil and mineral oils.

UNIT-II

INDUSTRIAL CHEMISTRY

Composition of soil - inorganic and organic components in soil- micro and macro nutrients. **Fertilizers:** Classification of Fertilizers- straight fertilizers, compound/complex fertilizers, fertilizer mixtures, manufacture and general properties of fertilizer products-Urea and DAP.

Ceramics: general properties, porous and non-porous wares, Manufacturing process, extrusion, turning, drying, decoration, Porcelain and china.

Cement: Types, manufacture, additives, setting, properties & testing of cement. **Glass:** Manufacture, properties, shaping of sheets & plate glasses. Annealing, finishing. special glasses.

Paints and Pigments: White pigments (white lead, ZnO, lithopone, titanium dioxide), blue, red, yellow and green pigments. paints and distempers, requirements of a good paint, emulsion, latex, luminescent paints, fire retardant paints, varnishes, enamels, lacquers, solvents and thinners.

UNIT-III

BIOORGANIC COMPOUNDS

Carbohydrates: Chemistry of important derivatives of monosaccharides - ethers, esters, acetals, ketals, deoxysugars and aminosugars.

Vitamins: Classification and Nomenclature. Source and deficiency diseases, biological functions of Vitamins- Vitamin A₂, Vitamin B, Vitamin C, Vitamin D & Vitamin K.

16 h

16 h

Food Analysis: Dairy products- composition of milk and milk products, analysis of fat content, minerals in milk and butter, Estimation of added water in milk.

Beverages: Analysis of caffeine in coffee and tea, detection of chicory in coffee, chloral hydrate in toddy, estimation of methyl alcohol in alcoholic beverages.

Food additives, adulterants and contaminants- Food preservatives like benzoates, propionates, sorbates, bisulphites, artificial sweeteners like saccharin, dulcin and sodium cyclamate.

Flavours: vanillin, esters (fruit flavours) and monosodium glutamate. Artificial food colourants - coal tar dyes and non-permitted colours and metallic salts. Pesticide residues in food.

Drugs: Classification and nomenclature. Analgesics - aspirin, paracetamol; Anthelmentics – mebendazole, Antiallergics - chloropheneramine malleate.

Antibiotics: Pencillin, chloromycetin and streptomycin.

UNIT-IV

16 h

INDUSTRIAL ORGANIC CHEMISTRY

Chemical energy systems and limitations, principles and applications of primary and secondary batteries and fuel cells, Basics of solar energy, Energy storage devices, Polymers in everyday life: from buckets to rockets: types and classification of polymers, source and general characteristics of natural and synthetic polymers, typical examples of polymers used as commodity plastics, textiles, electronic and automobile components, medical and aerospace materials, problems of plastic waste management, strategies for development of environmental friendly polymers.

Dyes:Colour and constitution (electronic concept). Classification of dyes, methods of applying dyes to the fabrics. A general study of Azo dyes, Orange –II, Mordant brown, Congo red and methyl orange.

Corrosion: Types and prevention, corrosion failure and analysis.

- 01. B.K. Sharma: introduction to Industrial Chemistry, Goel Publishing, Meerut(1998).
- 02. Medicinal Chemistry by Asthoush Kar.
- 03. Drugs and Pharmaceutical Sciences Series, Marcel Dekker, Vol.II, INC, New York.
- 04. Analysis of Foods H.E. Cox; 13. Chemical Analysis of Foods- H.E. Cox and Pearson.
- 05. Foods Facts and Principles. N. Shakuntala Many and S. Swamy, 4th ed. New Age Internatl (1998).
- 06. Physical Chemistry P. Atkins and J. de Paula -7 th Ed. 2002, Oxford University Press
- 07. Handbook on Fertilizer Technology by Swaminathan and Goswamy, 6 th ed. 2001, FAI.
- 08. Organic Chemistry by I. L. Finar, Vol. 1 & 2
- 09. Polymer Science and Technology, J. R. Fried (Prentice Hall)

III SEMESTER

CHIT- 3.1: INORGANIC CHEMISTRY-III

Teaching: 4 h/ week & Credits : 4

UNIT-I ELECTRONIC SPECTRA OF TRANSITION METAL COMPLEXES

Microstates, R-S coupling, term symbols for dⁿ ions, spectroscopic ground states, types of electronic spectra, selection rules for the electronic transitions, relaxation of the selection rules, nature of spectral bands, effect of spin-orbit coupling, effect of distortion and reduction in symmetry, Orgel diagrams, limitations of Orgel diagrams, Tanabe-Sugano diagrams, characteristics of the T-S diagrams, Racah parameters, interpretation of spectra of octahedral, tetrahedral, calculation of nephelauxetic parameter.

Charge transfer bands: origin, types and characteristics, intervalence charge-transfer bands. *Self study*: Prepare the chart for term symbols for dⁿ ions.

Skill component: Record the electronic spectra of transition metal complex (d^4 or d^7) and assign the bands.

UNIT-II

ORGANOMETALLIC CHEMISTRY-I

Classification of organometallic compounds, the 16 and 18 electron rule, synthesis, structure and bonding in metal alkyl (Li, Mg and Al) and reactions of Grignard's reagents.

Chemistry of organometallic compounds with π - bonding ligands: Synthesis, Structure, Spectroscopy, Reactions and bonding in metal – carbon π - bonded systems involving dihapto to hexahapto ligands viz, Olefins (Zeise's salt), allylic moieties, butadienes, cyclobutadienes and cyclopentadienes.

Fluxional behavior of organometallic compounds.

Homogeneous and heterogeneous catalysis: oxidative additions, reductive elimination, insertion and deinsertion reactions, hydrogenation, hydroformylation, isomerisation, carboxylation and polymerisation, water gas shift reaction.

Self study: Recent advance in fluxional behavior of organometallic compounds

Skill component: Preparation of any organometallic compound using Grignard's reagent.

UNIT-III 16 h **BIO INORGANIC CHEMISTRY: METAL STORAGE AND TRANSPORT**

Metal storage and transport of Fe, Zn, Cu, V, Mo, Co, Ni and Mn ions in living organism, iron proteins involved in transport and storage of iron (ferritin, hemosiderin, transferritin), copper proteins involved in transport and storage of copper (Ceruloplasmin serum albumin).

Electron transfer proteins - general features of iron sulfur proteins, Rubredoxin, Ferredoxins (2Fe-ferredoxin, Rieske proteins).

16 h

Total: 64 h

Blue-copper proteins: General features and types of blue copper proteins and their functions.

Cytochromes: structural features, classification and functions of cytochromes. Biological nitrogen fixation, *In vivo* and *in vitro* nitrogen fixation, Interactions of transition metal complexes with DNA.

<u>Self study</u>: Recent advances in electron transfer Fe-S proteins.

<u>Skill component:</u> Synthesis and characterization of metallo protein/ metallo enzyme /amino acid based metal complex.

UNIT-IV

16 h

BIO INORGANIC CHEMISTRY: METAL IONS IN BIOLOGICAL SYSTEMS

Essential and trace elements, biological functions of biometals, active transport of cations (Na and K pump), ionophores, different types of naturally occurring ionophores.

Metalloenzymes: metalloproteins as enzymes – carboxy peptidase, catalases, peroxidases, cytochrome P450, superoxide dismutase, copper oxidases, vitamin B12 coenzyme, synthetic model compounds.

Metals in medicine- metal deficiency (Fe, Mn, Cu and Zn), chelation therapy and metal complexes as drugs.

Chlorophyll and its role in photosynthesis: Transport and storage of dioxygen- heme proteins, oxygen uptake, functions of haemoglobin, myoglobin, hemerythrin and hemocyanins, synthetic oxygen carriers.

<u>Self study</u>: Functions of various metallo enzymes.

<u>Skill component</u>: Determination of metals in commercially available vitamin Tablets and /or preparation of salen-cobalt(II) complex and its oxygen scavenging activity.

- 01. Inorganic Chemistry: Principles, structure and reactivity, 1997, J.E. Huheey, Keiter and Keiter.
- 02. Inorganic Chemistry, 3rd edition, C. E. Housecroft and A. G. Sharpe.
- 03. Physical-Inorganic Chemistry; A coordination Approach by S. F. A. Kettle.
- 04. Inorganic Chemistry by Purcel and Kotz.
- 05. Inorganic Chemistry by W. W. Porterfield.
- 06. Concepts and Models of Inorganic chemistry by Douglass, Alexander and Mcdaniel.
- 07. Advanced Inorganic Chemistry by Cotton and Wilkinson.
- 08. Inorganic Chemistry by Miessler and Tarr.
- 09. Fundamental concepts of Inorganic Chemistry by A. K. Das, volume 1 to 7.
- 10. Electronic spectroscopy by D. N. Sathyanarayana.
- 11. Electronic Spectroscopy by A. B. P. Lever.
- 12. Elements of Magnetochemistry by Symal and Dutta.
- 13. Bioinorganic Chemistry by A. K. Das.
- 14. Bioinorganic Chemistry by Bertini, Gary, Lippard and Valentine

CHIPr -3.6: INORGANIC CHEMISTRY PRACTICAL-III

Duration: 4 h/ week & Total: 64 h

Credits : 2

PART-A Preparation of coordination compounds

- 01. Copper-glycine complex : cis and trans forms
- 02. Tris thiourea Copper (I) sulphate mono hydrate
- 03. Mercury tetrathiocyanatoCobaltate (II)
- 04. Tris ethylenediamine Ni(II) Chloride
- 05. Cis [Co(en)2Cl2] Cl
- 06. Separation of optical isomers of $[Co(en)3]^{3+}$

PART-B Characterization (Metal ion determination in above complexes

- 07. Copper by Iodometric method
- 08. Copper by Iodometric method
- 09. Nickel by gravimetric method
- 10. Cobalt volumetrically by EDTA method

PART-C Anion Estimation

- 11. SO4 ²⁻ as Barium Sulphate (gravimetrically)
- 12. Cl⁻ by Silver nitrate (demonstration)
- 13. Interpretation of IR and NMR Spectra of
- 14. Tris (thiourea) Copper (I) sulphate
- 15. Cis [Co(en)2Cl2]Cl
- 16. $[Co(en)3]^{3+}$

CHOT-3.2: ORGANIC CHEMISTRY-III

Teaching: 4 h/ week & Credits : 4

UNIT –I

REAGENTS IN ORGANIC SYNTHESIS

Use of the following reagents in organic synthesis and functional group transformation:

- 1. Gilmann reagent
- 3. Dicyclohexyl carbodimide (DCC)
- 5. Trimethylsilyl iodide
- 7. DDQ
- 9. Baker's Yeast
- 11. Crown ethers

- 2. Lithium diisopropyl amide (LDA)
- 4. 1,3-Dithiane (reactivity umpolung)
- 6. Tri-n-butyl tin hydride (TNBH)
- 8. Woodward-Prevost hydroxylation
- 10. Phase transfer catalysts
- 12. Peterson synthesis

<u>Self study(SS)</u>: Basics of reagents, storage, handling, expire date. Basic of Crown ethers and Phase transfer catalyst.

<u>Skill components(SC)</u>:Students need to list out hazardous and non- hazardous reagents in the above 12 synthesis. Give model for storing safe and handling during reaction (gaggle, Fume hood and other safety measures)

UNIT –II PHOTOCHEMISTRY

Interaction of radiation with matter, types of excitation, rate of excited molecules, quenching, quantum efficiency, quantum yield, transfer of excitation energy, actinometry, singlet and triplet states, experimental methods in photochemistry of carbonyl compounds, and transition, Norrish type I and Norrish type II reactions Paterno–Buchi reaction, photoreduction, photochemistry of enones, hydrogen abstraction rearrangement of unsaturated ketones and cyclohexadienones, photochemistry of parabenzoquinones, photochemistry of aromatic compounds with reference to isomerization, addition and substitution, photochemical isomerization of cis and trans alkenes, photo-Fries rearrangement, Barton reaction, Hoffmann- Loefler-Freytag reaction, photochemistry of vision.

<u>Self study(SS)</u>:Basics of photochemistry (PC), principle of PC, effect of photon on organic molecules.

Skill components(SC):Students select at least FOUR photoreaction products and analyse using different spectroscopic data (UV-Vis, FT-IR, NMR and mass spectrometry from online source).

UNIT –III

PERICYCLIC REACTIONS

Pericyclic Reactions: Classification of pericyclic reactions, molecular orbital symmetry, frontier orbitals of ethylene, 1,3-butadiene, 1, 3, 5-hexatriene, allyl system, Woodward-Hoffman correlation diagram method and Perturbation of molecular

16 h

16 h

16 h

Total: 64 h

orbital (PMO) approach of pericyclic reaction under thermal and photochemical conditions, FMO and PMO approach to the following reactions.

Electrocyclic reactions- Con rotatory and dis rotatory ring closure 4n and 4n+2 and allylic systems, Woodward and Hoffmann selection rules for pericyclic reactions.

Cycloadditions reactions - Antrafacial and suprafacial additions, more emphasis on [2+2] and [4+2] Cycloadditions, Diels-Alder reaction, 1,3-dipolar cycloaddition reactions.

Sigmatropic rearrangements: Antrafacial and suprafacial shift involving carbon moieties, retention and inversion of configuration, Ene, Claisen and Cope reaction.

<u>Self study(SS)</u>: Basics of pericyclic, elecctrocyclic and cycloaddition reactions. orbital shape, con-rotation and dis-rotation, stereochemistry.

<u>Skill components(SC)</u>:Students need to prepare some models (ball & Stick) to show some of the selected reactions.

UNIT –IV MEDICINAL CHEMISTRY

Basic consideration of drugs: Classification, nomenclature, metabolism and drug-receptor theory.

Synthetic drugs: Introduction, chemotherapy, pharmacodynamics, metabolites and antimetabolites, agonists and antagonists.

Antitubercular drugs - synthesis of isoniazide, p-amino salicylic acid and thiacetazone. Antineoplastic Agents: Introduction, cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechlorethamine, cyclophosphamide, mustards and mercaptopurine.

Cardiovascular drugs: Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output direct acting arteriolar dilators. synthesis of dithiazem, verapamil, atenolol, oxprenolol, antihypertensive drugs, lipid lowering agents (atorvastatin and statin derivatives).

<u>Self study(SS)</u>: Basic of drugs, chemotherapy, receptor, drug action and SAR studies. <u>Skill components(SC)</u>: Student need to list out stereochemistry and spectral data of UV-Vis, FT-IR and NMR of above class of pharmacological drug taken at least one drug.

REFERENCE BOOKS:

- 17. Fundamentals of photochemistry, K.K. Rohatgi Mukhergee, Wiley Eastern Limited, (1986)
- 18. Photochemistry, Carol E Wayne and Richard P Wayne, Oxford University Press, (1996)
- 19. Organic Photochemistry, J. M. Cozen and B. Halton, Cambridge University Press (I Edition) 1974

- 20. Molecular Reactions and Photochemistry, C H Deputy and D S Chapman, Prentice Hall India, New Delhi (1st Edition), 1972.
- 21. Concepts of Inorganic photochemistry, A. W. Adamson and P D Fleischaves Wiley.
- 22. Understanding organic reaction mechanisms, A. Jacob, Cambridge Univ. Press, 1997.
- 23. Introduction to organic chemistry A. Streitweiser, Jr and C. H. Heathcock, Macmillan, 1985.
- 24. Physical and mechanistic organic chemistry, R.A.Y. Jones, 1st Edn. Cambridge Univ. Press, 1979.
- 25. Mechanisms of molecular migrations, Vols I and II, B. S. Thiagarajan, 1st Edn. Pergamon Press, Oxford, 1979.
- 26. P. J. Garratt in Comprehensive organic chemistry, D. Barton and W. D. Ollis, 1st Edn. Pergamon Press, Oxford, 1979.
- 27. Radicals in organic synthesis, B. Giese, Pergamon Press, 1986.
- 28. Stereoelectronic effects in organic chemistry, P. Deslongchamps, 1st Edn. Pergamon Press, 1983.
- 29. Organic photochemistry, J. M. Coxon and B. Halton, 1st Edn, Cambridge Univ. Press, London, 1974.
- 30. Molecular reactions and photochemistry, C. H. Deputy and D. S. Chapman, 1st Edn. Prentice-hall India, New Delhi, 1972.
- 31. Burger's Medicinal Chemistry and Drug Discovery, Vols. 1-6 Ed. D.J. Abraham, John Wiley, 2003
- 32. Foye's Principles of Medicinal Chemistry, 6th Edn., T L Lemke and D A Williams Eds., Lippincott, Williams and Wilkins, 2007
- 33. An Introduction to Medicinal Chemistry, P Graham, III Ed., Oxford, 2006
- 34. Medicinal Chemistry, N Weaver, Oxford, 2006
- 35. Goodman and Gilman's Pharmacological Basis of Therapeutics, 11th Edn., Tata McGraw-Hill, 2005.
- 36. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical chemistry, J H Block and J M Beale, Jr., Eds., Lippincott, Williams and Wilkins, 2003.
- 37. Medicinal Chemistry G R Chatwal, Himalaya, New Delhi, 2002
- 38. Medicinal Chemistry, A Kar, Wiley, 2000.

CHOPr-3.7: ORGANIC CHEMISTRY PRACTICAL-III

Duration: 4 h/ week & Total: 64 h

Credits : 2

PART-A: ORGANIC ESTIMATIONS

- 01. Estimation of aniline
- 02. Determination of equivalent weight of acids by silver salt method.
- 03. Estimation of sugars by Fehling's method.
- 04. Determination of saponification value of oils.
- 05. Determination of iodine value of oils.
- 06. Determination of enol content by Meyer's method.

PART-B: MULTISTEP ORGANIC PREPARATION

- 01. Preparation of 2-bromo-3-phenyl propionic acid from cinnamic acid.
- 02. Preparation of anthralinic acid from phthalimide.
- 03. Preparation of p-chlorotoluene from p-toluidine.
- 04. Preparation of benzophenoneoxime and its rearrangement to benzanilide.

REFERENCES

- 01. Manual of Organic Chemistry, Dey and Seetharaman.
- 02. Modern experimental Organic Chemistry, John H. Miller and E. F. Neugil
- 03. An introduction to practical Organic Chemistry, Robert, Wingrove etc.
- 04. A Text book of practical Organic Chemistry, A I. Vogel Vol.III
- 05. Practical Organic Chemistry, Mann & Saunders
- 06. An Introduction to Practical Organic Chemistry, Robert, Wingrove etc.
- 07. Semimicro qualitative Organic Analysis, Cheronis, Entrikin and Hodnet
- Laboratory Manual of Organic Chemistry, R. K. Bansal New AGE International (P) Ltd. London, 3rd edition, 1996.
- 09. Practical Organic Chemistry, N.K. Visno, New AGE International(P) Ltd. London, 3rd edition, 1996.

CHPT-3.3: APPLIED PHYSICAL CHEMISTRY-III

Teaching: 4 h/ week & Credits : 4

UNIT-I

SUPERCONDUCTORS AND MEGNETOCHEMISTRY

Semiconductors: Free carrier concentration in semiconductors, Fermi level and carrier concentration in semiconductors, effect of temperature on mobility, electrical conductivity of semiconductors, Hall effect in semiconductors, p-n junction.

Superconductors: Introduction, conventional super conductors, magnetic properties of superconductors, The Meissner effect, Thermodynamics of superconducting transitions, London equation, London penetration Depth, Normal tunnelling and Josephson effect, BCS theory of superconductors, cooper pair, theory of high temperature superconductors and applications.

Magnetochemistry: Introduction, types of substances, theory of paramagnetism, diamagnetism and ferromagnetism (langevin's and Weiss's theory). Measurements of magnetic susceptibility: Theory of susceptibility, Gouy, Bhatnagar-Mathur and Quincke's method and applications of magnetic susceptibilities.

Skill development: Preparation of ferrites and study of magnetic properties.

UNIT-II

INTRODUCTION TO POLYMERS AND DENDRIMERS

Transition in Polymers: Definition of glass transition temperature (Tg) and flow temperature (Tf) and melting temperature (Tm). Comparison of Tg and Tm, Tg of copolymers and polymer blends, relation between Tg and Tm. Preparation, properties and commercial importance: polyethylene, polystyrene, polyvinyl chloride, poly sulphone, polyurethances, polyisoprenes. Metallocene catalysis polymerization (Ziegler-Natta polymerization). Ring opening metathesis polymerization. Commercial importance of cationic and anionic polymerization.

Biodegradable polymers: Chemical degradation, physical degradation, ageing, crazing, degradation by microorganisms, Biodegradable polymers, Mechanism of degradation, metal catalysed degradation.

Dendrimers and hyper-branched polymers: Introduction to dendrimers, Tecto- dendrimers. Structural of dendrimers (Compact nm-scale dendrimer structure, Dense presentation of multiple terminal groups and Core-shell molecular architecture).

Self-Study: Methods of preparation, common properties and applications. Skill development: Visiting polymer industries around Belgaum

UNIT-III CATALYSIS

Difference between heterogeneous, homogeneous and bio-catalysis; Importance of heterogeneous and homogeneous catalysis in chemical reactions, characteristics of catalytic reactions and acid-base catalysis.

Theories of Catalysis:, Boundary layer theory, Catalysis by semiconductors, Wolkenstein theory, Balanding's approach, electronic factors is catalysis by metals, molecular orbital approach.

Enzyme catalysis: Mechanism and kinetics of enzyme catalyzed reactions, the Michaelis-Menten equation, Effect of temperature on enzyme catalysis.

Heterogeneous catalysis: surface reactions, Kinetics of surface reactions, Unimolecular surface reactions, Bimolecular surface reactions, pH-dependence of rate constants of

16 h

16 h

Total: 64 h

catalyzed reactions, Autocatalysis and oscillatory reactions

Homogeneous Catalysis: Intermediate stages in homogenous Catalysis, energy profile diagram, general scheme for calculating kinetics of the reactions, decomposition of hydrogen peroxide, hydrogenation, hydroformulation, isomerization, wacker reaction, coupling reactions and asymmetric oxidations.

Skill development: Practical demonstrations and paper presentations.

UNIT-IV

SURFACE CHEMISTRY

Surface chemistry: Introduction, adsorption, isotherms(Gibbs, Frendlich, and Langmuir), surface excess; BET isotherm, surface area, pore size and acid strength measurement.LB film, membrane equilibrium, micellisation, catalytic activity, surface active agent, Classification of surface active agent, Critical Micellar Concentration (CMC), Factor affecting the CMC of surfactants, hydrophobic interaction, thermodynamics of micellization-phase separation and mass action model, micro emulsion, reverse miceles. Thermodynamics of adsorption: interpretation of chemisorptions based on the structure and nature. Kinetic of surface reactions: rate determining step, various types of reactions, Applications of adsorption:-High vacuum, Gas marks, Softening of hard water, Drying gases, Decolorisation, Refining of petroleum and vegetable oils, Prevention of evaporation of water. In curing diseases, concentration of ores, Adsorption indicators. **Skill development:**X-ray diffraction studies of oxides.

REFERENCE BOOKS:

- 1. G.C. Bond, —Heterogeneous catalysis and applications Oxford (1987)
- 2. D. K. Chakraborty and B. Vishwanathan, —Heterogeneous catalysis New Age (2008).
- 3. J. M. Thomas and W.J. Thomas —heterogeneous catalysis VCH publication (1997).
- 4. E. R. Rideal, —Concept in Catalysis Academic press (1968).
- 5. M. Beller, A. Renken and R. van Santen, —Catalysisl, Wiley VCH (2012).
- 6. G. Panchenov and V. Lebedev, —Chemical kinetics and catalysis Mir publication (1976).
- 7. S. J. Thomson and G. Webb, —Heterogeneous Catalysisl, Oliver & Boyd (1968).
- 8. R. Van Santen and J. Niemantsvedict, —Chemical Kinetics and Catalysis^{II}, Plenum Press (1995).
- **9.** D. Briggs and M. Seah, —Practical surface analysis by AES & XPSI, John Wiley (1983).

CHPPr-3.8: PHYSICAL CHEMISTRY PRACTICAL-III Duration: 4 h/ week & Total: 64 h Credits : 2

- 01. Analysis of binary mixture of two miscible liquids by viscometry and the relation between viscosity of solution and electrical conductivity
- 02. To determine the percentage composition of unknown mixture of A and B liquids by Abbe's refractometer by graphical method
- 03. To determine the percentage composition of unknown mixture of A and B liquids by Abbe's refractometer by formula method.
- 04. Determination of parachor value for CH2 groups by surface tension between two liquids 1) ethanol+propanol 2) ethanol+surfactant 3) propanol+surfactant.
- 05. To determine the step wise heat of neutralization of polybasic acid using thermoflask
- 06. Determine the concentration of Cu(II) and Fe(II) solution by photometric titration with EDTA
- 07. Determination of energy gap for semiconductor (Ge) and effect of temperature on semiconductor by four probe method.
- 08. Study of salt effect on solubility and determination of activity coefficient.
- 10. Adsorption: Invesitigation of adsorption of oxalic acid from aqueous solution by activated charcoal and examine the validity of Freundlich and Langmuir's adsorption isotherm.
- 11. Familiarity with word processing, Electronics spread sheets, Data processing, Mathematical packages, chemical structure drawing and molecular modeling.

Spectrophotometry:

- 1. Record the UV-spectra of a given compound, e.g. acetone in cyclohexane.
 - a. Plot transmittance versus wavelength
 - b. Plot absorbance versus wavelength
 - c. Calculate the energy involved in the electronic transition in different units, i.e,

cm⁻¹, J/mol, cal/mol and eV.

- 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.

Soft-core: CHGT- 3.4: SPECTROSCOPY-III

Teaching: 2 h/ week & Credits : 2

Total: 32 h

UNIT-I

ESR and Applications of IR Spectroscopy

Electron spin resonance (ESR) spectroscopy

Basic principle interaction between spin and magnetic field, origin of spectral lineintensity, width and position of spectral lines, relaxation process, multiplicity in ESR, hyperfine splitting, g-value and factor affecting. Rules for interaction of spectra, zero field splitting and Krammer's degeneracy, John-Teller distortion, isotropic and anisotropic coupling constants, nuclear quadrupole coupling interaction, spin hamitonium, ESR spectra of radical containing a single set of equivalent protons- methyl, parabezoquinone, cyclopentadienyl, benzene. ESR spectra of transition metal complexes, applications.

Applications of infra red spectroscopy to inorganic compounds

Infrared spectra of simple molecules and coordination compounds, changes in infrared spectra of donor molecules upon coordination (N,N-dimethylacetamide, urea, ammine, acetato, cyano and thiocyanato complexes), mono, di and trinuclear carbonyl complexes and nitrosyls complexes, change in spectra accompanying change in symmetry upon coordination (NO3⁻, SO4²⁻, NO2⁻ and ClO4⁻), hydrogen bonding, instrumentation including FTIR.

<u>Self study(SS)</u>: Basics of spins (Hunds rule, Aufbau principle), ESR, spectral line, magnetic field, diamagnetism and paramagnetism, degeneracy, rules for interaction of spectra.

<u>Skill components(SC)</u>: Analyze some important inorganic compounds (two samples in each) FT-IR and ESR spectra from open source/record spectra

UNIT-II NUCLEAR QUADRUPOLE RESONANCE and MOSSBAUER SPECTROSCOPY

Nuclear quadrupole resonance spectroscopy: Consequence of nuclear spin larger than ¹/₂, prolate and oblate nucleus, nuclear quadrapolar charge distribution-theory and instrumentation, relationship between electric field gradients and molecular structure, applications and interpretation of eQq data, effect of crystal lattice on the magnitude of eQq, structural information from NQR spectra.

Mossbauer spectroscopy: Theory and principles, experimental methods, isomer shift, quadrapole interactions, electron density, magnetic interactions; time and temperature dependent effect, application-Iodine trihalides, Prussian blue, trisiron dodecacarbonyl, tin halides, hexacyano ferrate and nitroprussides.

<u>Self study(SS)</u>: Basic of NqR and Mossbauer, prolate and oblate nucleus, electric field, electric field gradient, crystal lattice, electron density.

16 h

<u>Skill components(SC)</u>: Students need to prepare the model to show the working of Mossbauer spectroscopy experiment. Two complex sample Mossbauer spectra need to be analyzed from open source data.

REFERENCES

- Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash.
 4th edition, Tata McGraw-Hill, New Delhi.
- 15. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw-Hill, New York.
- 16. Introduction to Spectroscopy. Pavia, Lampman and Kriz, 3rd edition, Thomson.
- 17. Spectroscopy, B. P. Straughan and S. Walker, John Wiley & Sons Inc., New York, Vol. 1 & 2, 1976.
- 18. Vibration Spectroscopy Theory and Applications, D. N. Satyanarayana, New age International, New Delhi.
- 19. Organic Spectroscopy, William Kemp, 3rd edition, Palgrava, 1991.
- 20. Optical Method of Analysis, E. D. Olsen, McGraw Hill Inc, 1975.
- 21. Spectroscopy of organic compounds P. S. Kalasi, Wiley Eastern Ltd, India 1993.
- 22. Introduction to instrumental analysis R. D. Braun, McGraw Hill Book company 1982.
- 23. Physical methods in inorganic chemistry R. Drago, East West Pvt. Ltd, 1968.
- 24. Instrumental methods of chemical analysis Gurdeep Chatwal and Anand.
- 25. Organic Spectroscopy, 2nd edition– Jag Mohan, Narosa Publishing House New Delhi.
- 26. Applications of IR and Raman spectroscopy to coordination and organometallic compounds, K. Nakamoto.

[OPEN ELECTIVE]

CHEG-3.5: ENVIRONMENTAL CHEMISTRY

Teaching: 4 h/ week & Credits : 4

UNIT-I POLLUTION

Environmental segments, evolution of earth's atmosphere.

Air pollution: Air pollutants, prevention and control, green house gases and acid rain, carbon monoxide, industrial sources and transportation sources.

 SO_{x} - sources, ambient concentration, test methods, control techniques - scrubbing, , limestone injection process. Ozone hole and CFC's, photochemical smog and PAN. NO_{x} - sources, ambient concentration, test methods, thermodynamics and NO_{x} , control techniques.

Particulates: Size distribution, particulate collection - settling chambers, centrifugal separators, wet scrubbers, electrostatic precipitators & fabric filters, catalytic converters for mobile sources, Bhopal gas tragedy.

UNIT-II

WATER POLLUTION

Hydrologic cycle, sources, chemistry of sea water, criteria and standards of water quality- safe drinking water, maximum contamination levels of inorganic and organic chemicals, radiological contaminants, turbidity, microbial contaminants, public health significance and measurement of colour, turbidity, total solids, acidity, alkalinity, hardness, chloride, residual chlorine, sulphate, fluoride, phosphate and different forms of nitrogen in natural and polluted water, chemical sources of taste and odour, treatment for their removal, sampling and monitoring techniques.

UNIT-III

WATER ANALYSIS

Determination and significance of DO, BOD, COD and TOC, water purification for drinking and industrial purposes, disinfection techniques, demineralization, desalination processes and reverse osmosis.

Radioactive waste management, radionuclides in soil, effects of ionizing radiationseffect on ecosystem, accidents at atomic power plants-Chernobyl disaster, disposal of radioactive liquid wastes, methods of radiation protection.

UNIT-IV

DETERGENTS, PESTICIDES and SOIL ANALYSIS

Toxic chemicals in the environment, impact of toxic chemicals on enzymes. **Detergents**- pollution aspects, eutrophication.

Pesticides-pollution of surface water. Sewage and industrial effluent treatment, heavy metal pollution. Chemical speciation- biochemical effects of pesticides, insecticides, particulates, heavy metals (Hg, As, Pb, Se), carbon monoxide, nitrogen oxides, sulphur oxides, hydrocarbon, particulates, ozone, cyanide and PAN. Solid pollutants and its treatment and disposal.

16 h

16 h

Total: 64 h

16 h

Composition of soil - Inorganic and organic components in soil, micro and macro nutrients, nitrogen and sulphur pathways, soil pollution: classification of pollutants and their characteristics, sources, prevention and control, sampling and monitoring techniques.

- 01. A.K. De : Environmental Chemistry (Wiley Eastern).
- 02. S.K. Banerji : Environmental Chemistry (Prentice Hall India), 1993.
- 03. S.D. Faust and O.M. Aly : Chemistry of Water Treatment, (Butterworths), 1983.
- 04. G.D. Christian : Analytical Chemistry, (4th Ed.), (John Wiley)
- 05. Sawyer and McCarty, Chemistry for Environmental Engineering (McGraw Hill) 1978
- 06. I. Williams, Environmental Chemistry, John Wiley, 2001
- 07. S. M. Khopkar, Environmental Pollution Analysis, (Wiley Eastern).
- 08. J.W. Moore: Heavy Metals in Water, (Springer-Verlag), 1984.
- 09. C. Malcolm, K.Killham and Edwards: Soil Chemistry and its Applications, Cambridge (1993)
- 10. M. Raymond and J.C. Shickluna: Soils, 5th Ed. (Prentice Hall, India), 1987.

IV SEMESTER

CHIT-4.1: INORGANIC CHEMISTRY-IV

Teaching: 4 h/ week & Credits : 4

UNIT-I

NON-TRANSITION, F-BLOCK ELEMENTS & CARBENES

Silicates: Types of silicates, Clay minerals and Zeolites

Phosphazenes: Synthesis of Cyclophosphazenes and polyphosphaznes. Reactions of Hexachlorocyclotriphosphazene and polyphospazne. Structural aspects of Hexachlorocyclotriphosphazene.

Sulphur-Nitrogen compounds: Synthesis, structure and reactivity of S4N4, S4N4H4, S2N2 /and (SN)x.

Carbenes: Singlet and triplet state, Fisher and Schrock carbenes, metal carbenes, reactivity of carbenes and metal carbenes.

Chemistry of f-block metals: f-orbitals and oxidation states, atom and ion sizes, spectroscopic and magnetic properties (Electronic spectra and magnetic moments of lanthanides, luminescence of lanthanide complexes, Electronic spectra and magnetic moments of actinides), inorganic compounds and coordination complexes of the lanthanides and uranium.

Self study: Synthesis and structural aspects of Uranium complexes. Skill component: Collection of Montmorillonite (2:1 smectite) clay mineral from soil.

UNIT-II

MATERIAL CHEMISTRY

Fuel Analysis: Definition and classification of fuels, characteristics of fuels, sampling, proximate and ultimate analysis of coal, and determination of calorific value. Liquid fuels: determination flash point, fire point, aniline point, knocking of petrol and diesel octane and cetene numbers, carbon residue.

Gaseous fuels: Analysis of coal gas, water gas, producer gas, gobar gas and blast furnace gas. Calorific value, determination of Junker's gas calorimeter. Relative merits of solid, liquid and gaseous fuels.

Explosives: TNT, RDX etc.

Metal hydrides and Carbides: Salt like, covalent and interstitial carbides, Metal hydrides relevant to hydrogen storage applications (NaH, NaBH4, LiAlH4 etc.)

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.

Self study: Chemical weapons and their impact on mass destruction - safety issues.

16 h

16 h

Total: 64 h

<u>Skill component</u>: Determination of calorific value of any suitable fuel or Preparation of silicone polymer.

UNIT-III

SOLID STATE CHEMISTRY

Electrical properties of solids: Conductors, insulators, semiconductors. Measurements by DC and AC methods.

Ionic conductivity: Alkali halides- vacancy conduction in NaCl crystal, interstitial conduction in AgCl.

Li-ion battery – Electrode materials and working.

Solid electrolytes: β - Alumina, AgI and Ag+ ion solid electrolytes, anion conductors (Yttria stabilized zirconia), requirements for conductivity, Applications including solid oxide fuel cell.

<u>Self study</u>: Cathode materials used in Li-ion battery.

<u>Skill component</u>: Deduce the ionic conductivity of anion conductor (YSZ) from the Nyquist plot.

UNIT-IV MAGNETIC & OPTICAL PROPERTIES

Magnetic properties: Types of magnetic materials (magnetic ordering in Ferro, antiferro, dia, para and ferri). Magnetically concentrated compounds- ferro, antiferro and ferri magnetic, spin cross-over systems.

Magnetization vs. applied field(hysteresis loops), Effect of temperature, spin-only formula, orbital contribution, spin-orbit coupling.

Selected examples of magnetic materials (Fe2O3, Fe3O4), metal and alloys, transition metal oxides, spinels, garnets, ilemenites, perovskites, magneto plumbites.

Measurement of magnetic susceptibility – Gouy and Faraday methods, diamagnetic corrections. correlation of magnetic and structural properties, applications.

Optical properties: Luminescence and phosphors, configurational coordinate model, some phosphor material, antistokes, phosphors, lasers.

<u>Self study</u>: Different types of magnetic materials – effect of temperature.

<u>Skill component</u>: Determine the magnetic susceptibity of any transition metal and/or Lanthanide complex by Guy's method.

REFERENCE BOOKS:

- 01. Inorganic Chemistry: Principles, structure and reactivity, 1997, J.E. Huheey, Keiter and Keiter.
- 02. Inorganic Chemistry, 3rd edition, C. E. Housecroft and A. G. Sharpe.
- 03. Inorganic Chemistry by Purcel and Kotz.
- 04. Inorganic Chemistry by W. W. Porterfield.
- 05. Concepts and Models of Inorganic chemistry by Douglass, Alexander and Mcdaniel.
- 06. Advanced Inorganic Chemistry by Cotton and Wilkinson.

16 h

- 07. Inorganic Chemistry by Miessler and Tarr.
- 08. Fundamental concepts of Inorganic Chemistry by A. K. Das, volume 1 to 7.
- 09. Elements of Magnetochemistry by Symal and Dutta.
- 10. Organometallic Chemistry by Meharotra and Singh.
- 11. Organometallic Chemistry by G. E. Coates.
- 12. Introduction to Solids by Azaroff.
- 13. Solid State Chemistry and its Applications by Anthony R. West.
- 14. Solid State Chemistry: An Introduction, 3rd edition, Lesley E. Smart and Elaine A. Moore.

CHIPr -4.6: INORGANIC CHEMISTRY PRACTICAL-IV Duration: 4 h/ week & Total: 64 h Credits : 2

- 01. Use of Cation and Anion resins column set up.
- 02. Analysis of Cement (SO3).
- 03. Use of oxime, salicyladoxime, DMG in the separation and estimation using spectrophotometric/volumetric/gravimetric method.
- 04. Cu + Ni
- 05. Al + Mg
- 06. Ni in the presence of Fe.

CHOT-4.2: ORGANIC CHEMISTRY-IV

Teaching: 4 h/ week & Credits : 4

Total: 64 h

16 h

UNIT –I ORGANIC SYNTHESIS

Designing the synthesis based on retrosynthetic analysis

Disconnection Approach: An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclization reactions, amine synthesis.

One Group C-C Disconnections: Alcohols and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes in organic synthesis.

Two Group C-C Disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, α , β -unsaturated carbonyl compounds, Michael addition and Robinson annulations.

Retrosynthesis: Retrosynthesis of benzocaine, 4-methoxy acetophenone, saccharin and bisavalone.

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

<u>Self study(SS)</u>:Basic of retrosynthetic analysis, synthons, synthetic equivalents, chemoselectivity, reversal of polarity, cyclization reactions, basic of protecting group.

<u>Skill Components (SC)</u>: Student need to analyse retosynthetic pathways of saccharin and acetophenone product and intermediate analysis using several spectral data. How carbonyl group is protection monitored by FT-IR spectra need to be explained by taking (acetal and cyclic acetal formation one reaction)

UNIT-II: BIOORGANIC POLYMERS

16h

Biopolymers: Biological importance of cellulose, starch, glycogen, dextran, hemicellulose, pectin, agar-agar, and industrial importance of cellulose.

Lignin: Different process of isolation, structure, importance of delignification in paper industry, biodegradation of lignins.

Peptide and Proteins: Introduction peptides, use of N- and C-blocking agents, Chemical synthesis of peptides (acid chloride, DCC and mixed anhydride method), Solid phase - Merrifield synthesis.

Proteins: End group analysis (Sangers and Edmans), isolation, purification and classification, primary, secondary and tertiary structure, denaturation and renaturation, biological and industrial importance of silk, and casein.

Nucleic Acids: Introduction, classification, components of nucleic acids, nucleosides and nucleotides, Watson-Crick model of DNA, and applications of RNA and DNA.

<u>Self study(SS)</u>:Basics of carbohydrates, origin, types, examples, stereo isomers of D-Glucose, Basic chemistry of amino acids, types of amino acids, history of nucleic acids. <u>Skill components</u>: Students need to analyse spectral data of D- Glucose and D-Fructose(open source/record). Pentapeptide sequence (H2N-Leu-Ala-Phe-Pro-Gly- OH)

analyzed mass spectrometry fragmentation pattern and confirm the sequence. DNA and RNA mass determination techniques may be model/analyzed (open source).

UNIT –III

ALKALOIDS AND TERPENOIDS

Alkaloids: Introduction, classification, methods of isolation, general methods of isolation from plants, general methods of structural elucidation, structural elucidation and synthesis of ephedrine and quinine. Structure and biological importance of cocaine, codaine, thiebane and morphine.

Terpenoids: Introduction, classification, isoprene rule, structural elucidation and synthesis of menthol and zinzeberine.

Antibiotics: Introduction, classification, structure and their importance of penicillins, chloramphenicol, streptomycine, chloromycitin and tetracyclins, synthesis of cepahloshorin-C.

<u>Self study(SS)</u>:Basics of alkaloids, terpenoids and antibiotics, isolation and nomenclature.

<u>Skill components(SC):</u> Analyzeeach one compound of the above class using various spectra.

UNIT –IV

STEROIDS, ANTIBIOTICS AND PROSTAGLANDINS

Steroids: Introduction, classification; Diels hydrocarbon- its importance and synthesis, stereochemistry of cholesterol.

Structural elucidation of cholesterol-Blanc's rule, location of double bond, hydroxy group, angular methyl groups and side chain in cholestrerol, total synthesis.

Prostaglandins: Introduction, classification and biological importance, constitution of PGE1, synthesis of PGE1 by Corey's and Upjohn's approach.

Vitamins: Definition, Classification and biological importance, synthesis of vitamin C from D(+)-Glucose, synthesis of vitamin A.

<u>Self study(SS)</u>: Basics of steroids , Prostaglandins, Vitamins, occurrence, nomenclature and isolation.

<u>Skill components(SC)</u>:Students can make model of cholesterol.Students need to perform a small group project on water soluble & fat soluble vitamins, and analyze Vit- A UV-vis and FT-IR data (record/open source).

REFERENCE BOOKS:

- 01. F. A. Carey and Sundberg, Advanced Organic Chemistry Part A & B, 3rd edition, Plenum Press, New York, 1990.
- 02. F. A. Carey and Sundberg, Advanced Organic Chemistry Part A & B, 3rd edition, Plenum Press, New York, 1990.
- 03. Comprehensive Organic Synthesis B. M. Trost and I. Fleming series, Pergamon Press, New York, 1991.
- 04. S. K. Ghosh, Advanced General Organic Chemistry, Book and Alleied (P) Ltd, 1998
- 05. Principles of organic synthesis, Richard Norman and J. M. Coxon

16 h

- 06. Disconnection approach, by Steurt Warren.
- 07. Natural products: Their chemistry and biological significance-J. Mann,
- 08. R. S. Davidson, J. B. Hobbs, D. V. Banthorpe& J. B. Harborne, Longman, UK,

- 10. Terpenes, J. Verghese, Tata McGraw-Hill, New Delhi, 1982.
- 11. Chemistry of terpenes and terpenoids, A. Newman, Academic Press, London, 1975.
- 12. 4. Handbook of naturally occurring compounds Vol. II: Terpenes, T. K. Davon, I. Scott, Academic Press, NY, 1972.
- Natural products chemistry Vol. I & II, K. Nakanishi, T. Goso, S. Ito, S. Natori & S. Nozoe, Academic Press, NY, 1974.
- 14. Total synthesis of natural products Vol. I & VI, Apsimon, John Wiley, NY, 1973-1981.
- 15. Organic chemistry Vol.II, I. L. Finar, 6thEdn. Longman,1992.
- 16. Chemistry of natural products Vol. I & II, O. P. Aggarwal, Goel Publishing House, 6thEdn. 1982.
- 17. Total synthesis of natural products: The chiral approach Vol.III, S. Hanessian
- 18. Pergamon Press, 1983.
- 19. Total synthesis of steroids, Akhaun&Titov, Jerusalem, 1969.
- 20. Medicinal natural products: A biosynthetic approach, P. M. Dewick. John Wiley, Chichester, 1997.
- 21. The colours of life: An introduction to the chemistry of porphyrins and related compounds, L. R. Milgrom, Wiley Chichester, 1995.
- 22. Spectral data of natural products Vol. I- K.Yamaguchi, Elsevier Publishing Co, London,1970.
- 23. Chemistry of natural products: A unified approach, N. R. Krishnaswamy, University Press, India, 1999.

^{09. 1994.}

CHOPr-4.7: ORGANIC CHEMISTRY PRACTICAL-IV Duration: 4 h/ week & Total: 64 h Credits : 2

PART-A : Isolations

- 01. Isolation of cysteine from human hair
- 02. Isolation of hesperidine from orange peel
- 03. Isolation of myristine from nutmug
- 04. Isolation of lycopene from tomato
- 05. Isolation of piperine from pepper
- 06. Isolation of caffeine from tea
- 07. Isolation of casein from milk
- 08. Isolation of nicotine from tobacco

PART-B : INSTRUMENTAL METHODS IN ORGANIC ANALYSIS

- 01. Recording/predicting/downloading from web sites the UV, IR, NMR and GC-MS/mass spectra of the compounds prepared in C-105/205/305 (Organic Practical I), C-106/206/306 (Organic Practical II), C-405 (Organic Practical III) and C-406 (Organic Practical IV).
- 02. Structural elucidation of organic compounds with the help of spectra provided by the instructors/examiners.

- 01. Manual of Organic Chemistry Dey and Seetharaman.
- 02. Modern experimental Organic Chemistry John H. Miller and E. F. Neugil
- 03. An introduction to practical Organic Chemistry Robert, Wingrove etc.
- 04. A Text book of practical Organic Chemistry A I. Vogel Vol.III
- 05. Practical Organic Chemistry Mann & Saunders
- 06. An Introduction to Practical Organic Chemistry Robert, Wingrove etc.
- 07. Semimicro qualitative Organic Analysis Cheronis, Entrikin and Hodnet
- 08. Laboratory Manual of Organic Chemistry R. K. Bansal New AGE International (P) Ltd. London, 3rd edition, 1996.
- 09. Practical Organic Chemistry N. K. Visno, New AGE International(P) Ltd. London, 3rd edition, 1996.

CHPT-4.3: APPLIED PHYSICAL CHEMISTRY-IV

Teaching: 4 h/ week & Credits : 4

UNIT-I

PARTIAL MOLAR PROPERTIES

Partial molar properties, concept of partial molar properties, consequences of partial molar property concept. Physical significance of partial molar quantities. Determination of partial molar properties (direct method, intercept method, apparent molar properties). Chemical potential, physical significance of chemical potential, variation of chemical potential with pressure and temperature. Gibb's Duhem equations, chemical potential of a pure solid or liquid. Chemical properties of pure ideal gas, non ideality, activity, fugacity, activity coefficients for solutes and solvents. Determination of activity coefficient, thermodynamic function of ideal

gases i) free energy of ideal mixing ($\Box G \min x$) ii) enthalpy of ideal mixing iii) entropy of ideal mixing iv) volume of ideal mixing v) Helmholtz's free energy of ideal mixing vi) Duhem-Margules equation and its applications. Thermodynamics of ideal and non ideal solutions. Relationship between chemical potential Kapler-Clausius equation. **Skill development:** Formal Report on Partial Molar Volume Experiment

UNIT-II

NANOMATERIALS & LIQUID CRYSTALS

Mesomorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases; smectic – nematic transition and clearing temperature- homeotropic, planar and schlieren textures, twisted nematics chiral nematics, molecular arrangements in smectic A & C phases. Optical properties of liquid crystals.

Nanomaterials: Introduction – importance and characterization of nanomaterials – stability of nanoparticles In solutions – synthesis of metal nanomaterials: Physical methods (Laser Ablation, Evaporation, sputtering and solvated metal dispersion) chemical methods (Thermolysis, Sonochemical approach, reduction of metal ions by hydrogen and methanol)

Skill development: Synthesis of nanomaterials by chemical method.

UNIT-III CHEMICAL KINETICS

Kinetics of opposed reactions, 1st order opposed by 1st order, 1st order opposed by 2nd order. 2nd order opposed by 2nd order. Kinetics of parallel and simultaneous reactions,(derivation of rate equations), time for maximum concentration of intermediate, Kinetics of chain reactions, activation energy of chain reactions, chain length, chain transfer reactions, inhibition decomposition of C2H6, Reaction between H2 with Br2 and Cl2, decomposition of O3, Rice-Herzfeld mechanism with example(CH3CHO), polymerization reactions. Kinetics of polymerization reactions, free-radical mechanism, kinetics of addition polymerization,

Skill development: Literature survey of chemical kinetics.

Total: 64 h

16 h

16 h

UNIT-IV

ELECTROCHEMISTRY AND ELECTROPLATING ELECTROCHEMISTRY AND ELECTROPLATING

Batteries: An electrochemical source of energy, Types of Batteries: - Primary, and Secondary batteries. Dry cell, Lead acid storage cell, Nickel/Cadmium battery fundamentals of Lithium-ion battery construction and working principle. Fuel cell- definition example H2/O2 fuel cell [green fuel cell] - solar cells.

CORROSION AND PLATING: Types, measurement and preventive methods, metallic and non metallic coatings. Corrosion inhibition. Measurement of corrosion rate by weight loss, Tafel plots. Homogeneous theory of corrosion. Evans diagrams. Potential- pH (Pourbaix) diagrams of iron. Metal finishing, electroplating of single metals like Zn, Cd, Cu, Au, Pt- alloy plating, industrial application.

Skill development: Electrodeposition of Zn and Cu from different alkaline bath solutions.

- 01. Elements of statistical thermodynamics- E.K.Nash, Wesley, 1974
- 02. Statistical thermodynamics- M.C.Gupta, Willey Eastern ltd. 1990.
- 03. Statistical mechanics-Doley.
- 04. Textbook of polymer science –Billmeyer, Willey Intersection.
- 05. Elements of statistical thermodynamics- E.K.Nash, Wesley, 1974
- 06. Statistical thermodynamics- M.C.Gupta, Willey Eastern ltd. 1990.
- 07. Statistical mechanics-Doley.
- 08. Introduction to Solid state Physics—C. Kittel, 5th Edition, Wiley Eastern, Limited.
- 09. C.N.R. Rao and J. Gopalakrishna —New Directions in solid state chemistry Cambridge University Press, Cambridge (1999).
- 10. Electrochemistry –Principles and applications by E.G. Potter.
- 11. Electrochemistry by Reiger, Prentice Hall (1987).

CHPPr-4.8: PHYSICAL CHEMISTRY PRACTICAL-IV Duration: 4 h/ week & Total: 64 h Credits : 2

Chemical Kinetics

- 1. Kinetics of acid catalyzed hydrolysis of methyl acetate and determination of energy of activation.
- 2. Kinetics of reaction (second order) between K₂S₂O₈ versus KI) and study of effect of ionic strength in media.

Partial Molar properties:

1. Partial Molar volume of ethanol-water system by intercept method.

Electoplating:

- 1. Electro deposition of copper by deposition method.
- 2. Corrosion of an electrode by weight loss method.

Semi Conductors:

1. To calculate the band gap energy (E_g) in semiconductors

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

Soft-core: CHGT-4.4: SPECTROSCOPY-IV

Teaching: 2 h/ week & Credits : 2

Total: 32 h

UNIT-I

AAS and CHIROPTICAL SPECTROSCOPY

Atomic Absorption Spectroscopy (AAS): Introduction, atom and atomic spectroscopy, basic principle, instrumentation (single and double beam), light source, measurement, analytical, chemical interference, spectral interference (Continuum Source Background Correction and Zeeman Background correction), advance AAS techniques recent development and applications.

Chiroptical spectroscopy: Plane polarized light, optical rotary dispersion (ORD), instrumentation, plane curves, Cotton effect curves, application of optical rotation method in the determination of rate constants, acid catalyzed muta-rotation of glucose, and inversion of cane sugar, octant and haloketone rules. Applications of ORD in the determination of configuration of cyclic steroidal ketones.

<u>Self study (SS):</u> Basic of atomic spectra, Polarized light, optical activity, specific rotation. <u>Skill components(SC):</u>Students need to analyze one ORD spectrum of steroid stereochemistry and two halo ketone compounds (open source) and simple structure model may be constructed.

UNIT-II

16 hours

MOLECULAR LUMINESCENCE and PHOTOELECTRON SPECTROSCOPY Molecular luminescence spectroscopy: Theoretical basis for fluorescence andphosphorescence. Singlet and triplet excited states. Variables affecting luminescence-

quantum efficiency, transition types, structure and structural rigidity, temperature and solvent effects, effect of pH, dissolved oxygen and concentration effect. Excitation spectra *vs* emission spectra. Fluorescence instrumentation- fluorometers and spectrofluorometers. Sensitivity and selectivity. Modification necessary to measure phosphorescence. General scope of applications of luminescence.

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

<u>Self study(SS)</u>:Basic of fluorescence and phosphorescence, singlet and triplet states, photo-ionization process, chemical shifts and basic of photoelectron spectra.

<u>Skill components(SC)</u>: Students need to list out THREE molecule fluorescence spectra and analyze. Students need to collect N2, NaN3 and HBr molecules photoelectron spectra (open source) and analyze.

REFERENCE BOOKS:

01. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash. 4th edition, Tata McGraw-Hill, New Delhi.

- 02. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw-Hill, New York.
- 03. Introduction to Spectroscopy. Pavia, Lampman and Kriz, 3rd edition, Thomson.
- 04. Spectroscopy, B. P. Straughan and S. Walker, John Wiley & Sons Inc., New York, Vol. 1 & 2, 1976.
- 05. Vibration Spectroscopy Theory and Applications, D. N. Satyanarayana, New age International, New Delhi.
- 06. Organic Spectroscopy, William Kemp, 3rd edition, Palgrava, 1991.
- 07. Optical Method of Analysis, E. D. Olsen, McGraw Hill Inc, 1975.
- 08. Spectroscopy of organic compounds P. S. Kalasi, Wiley Eastern Ltd, India 1993.
- 09. Introduction to instrumental analysis R. D. Braun, McGraw Hill Book company 1982.
- 10. Physical methods in inorganic chemistry R. Drago, East West Pvt. Ltd, 1968.
- 11. Instrumental methods of chemical analysis Gurdeep Chatwal and Anand.
- 12. Organic Spectroscopy, 2nd edition– Jag Mohan, Narosa Publishing House New Delhi.
- 13. Applications of IR and Raman spectroscopy to coordination and organometallic compounds, K. Nakamoto.

Question paper Pattern of 4 Credit Paper

II Semester (Regular/ Repeater) M.Sc. Degree (CBCS) Examination, June/July-20xx CHEMISTRY Paper CHIT-2.1: Inorganic Chemistry-II

Time : 3 Hours

Max. Marks : 80

Instructions: Answer all questions

1.		Answer any eight of the following q	uestions.	(8x2 = 16)
	a)			
	b)			
	c) d)			
	u) e)			
	f			
	g)			
	h)			
	i)			
	j)			
\mathbf{r}	a)			
4.	a) b)			
	c)			
			OR	
	d)			(5+5+6)
2	`			
3.	a) b)			
	c)			
	•)		OR	
	d)			(5+5+6)
4.	a)			
	b)			
	0)		OR	
	d)		OIX .	(5+5+6)
5.	a)			
	b)			
	c)		OD	
	d)		UK	(5+5+6)
	u)			(3+3+0)

Question paper Pattern of 2 Credit Paper

II Semester (Regular/ Repeater) M.Sc. Degree (CBCS) Examination, June/July-20xx CHEMISTRY Paper CHGT-2.4: Spectroscopy-II

Max. Marks : 40

Time : 2 Hours

Instructions: Answer all questions						
1. a) b) c) d) e) f)	Answer any four of the following questions.	(4x2 = 8)				
2. a) b) c) d)	OR	(5+5+6)				
3. a) b) c) d)	OR	(5+5+6)				
