

No. BCU/BoS/Chemistry /47/2020-21.

Date. 31.07.2020.

**NOTIFICATION**

Sub: Revised Syllabus for Chemistry 3<sup>rd</sup> & 4<sup>th</sup> Semester of Bengaluru Central University.

- Ref: 1. First and Second Semester Revised Syllabus Notification No: BCU / BoS/Chemistry/210/2019-20 dated 11.07.2019.  
2. The recommendations of the Board of Studies in Chemistry (PG).  
3. Approval of the Academic Council at its meeting held on 30.05.2020.  
4. Orders of the Vice-Chancellor dated 29.07.2020.

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In pursuance to the recommendations of the Board of Studies in Chemistry (PG) and approval of the Academic Council, cited at reference above, the revised Syllabus for Chemistry 3<sup>rd</sup> and 4<sup>th</sup> Semester of Bengaluru Central University is hereby notified for implementation from the academic year 2020-21.

The copy of the Syllabus is notified in the University Website: [www.bcu.ac.in](http://www.bcu.ac.in) for information of the concerned.

  
REGISTRAR

To,

1. The Dean, Faculty of Science, BCU.
2. The Chairman & Members of BoS in Chemistry (PG) , BCU.
3. The Principals of the concerned affiliated Colleges of BCU – through email.
4. The P.S. to Vice-Chancellor/Registrar/Registrar (Evaluation), BCU.
5. Office copy / Guard file.



**M. Sc., Chemistry (CBCS)**

**Syllabus**

**(w. e. f. 2019-2020)**

**Department of Post-Graduate Studies in Chemistry**  
Central College Campus  
Palace Road  
Bengaluru – 560 001.

### SYLLABUS 2019-20

- |                           |   |   |
|---------------------------|---|---|
| 1. Name of the Course     | : | <b>M.Sc., Chemistry</b>   |
| 2. Duration of the Course | : | Two Years (FOUR SEMESTERS, CBCS)  |
| 3. Eligibility            | : | A candidate must have secured 40% marks in the aggregate and studied Chemistry (cognate subject) securing 50 % marks in this subject at the B Sc., level and studied Mathematics at 10 + 2 or Pre-university level. |
| 4. Intake                 | : | 40 + Supernumerary seats + Payment  |
| 5. Admission              | : | seats= 60 (Total)   |
|                           | : | As per University regulations   |

## I Semester

Code No	Title	Theory/ Practical (Hrs/ Week)	Total No. of Hrs/ Semester	Duration of Exam. Hours	Max. Marks (Exam)	Continuous Evaluation	Total Marks	Credits
Ch-101	Inorganic Chemistry-I	4	52	3	70	30	100	4
Ch-102	Organic Chemistry-I	4	52	3	70	30	100	4
Ch-103	Physical Chemistry-I	4	52	3	70	30	100	4
Ch-104	Analytical Chemistry	4	52	3	70	30	100	4
Ch-105	Mathematics for Chemists (Soft Core)	3	36	3	70	30	100	2
Ch-106	Practical-I Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-107	Practical-II Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-108	Practical-III Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-109	Practical-IV Inorg/Org/Phy	4	60	4	35	15	50	2
							700	26

### Scheme for continuous evaluation

#### A. Theory (each paper)

Tests\* :30 Marks

- \* Two tests will be conducted and the average marks of the two tests will be taken for Internal assessment.

#### B. Practical: 30 marks for experiment + 5 marks for Viva-Voce

IA : 15 Marks (based on Test + Record)

  
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## II Semester

Code No	Title	Theory/ Practical (Hrs/ Week)	Total No.of Hrs/ Semester	Duration of Exam. Hours	Max. Marks (Exam)	Continuous Evaluation	Total Marks	Credits
Ch-201	Inorganic Chemistry-II	4	52	3	70	30	100	4
Ch-202	Organic Chemistry-II	4	52	3	70	30	100	4
Ch-203	Physical Chemistry-II	4	52	3	70	30	100	4
Ch-204	Molecular Spectroscopy	4	52	3	70	30	100	4
Ch-205	Green Chemistry/ Photo Chemistry (Soft Core)	3	36	3	70	30	100	2
Ch-206	Practical-I Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-207	Practical-II Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-208	Practical-III Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-209	Practical-IV Inorg/Org/Phy	4	60	4	35	15	50	2
							700	26

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#### B. Practical: 30 marks for experiment + 5 marks for Viva-Voce

IA : 15 Marks (based on Test + Record)

  
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**M. Sc. Chemistry (Inorganic Specialisation)  
III Semester**

Code No	Title	Theory/ Practical (Hrs/ Week)	Total No. of Hrs/ Semester	Duration of Exam. Hours	Max. Marks (Exam)	Continuous Evaluation	Total Marks	Credits
Ch-301 IC	Inorganic Reaction Mechanisms and Bioinorganic chemistry	4	52	3	70	30	100	4
Ch-302 IC	Advanced Analytical Techniques	4	52	3	70	30	100	4
Ch-303 IC/OC/PC	Organic Spectroscopy	4	52	3	70	30	100	4
Ch-304 OE	Open Elective	4	52	3	70	30	100	4
Ch-305	Practical-I Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-306	Practical-II Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-307	Practical-III Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-308	Practical-IV Inorg/Org/Phy	4	60	4	35	15	50	2
							600	24

**Scheme for continuous evaluation**

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**M. Sc. Chemistry (Inorganic Specialisation)  
IV Semester**

Code No	Title	Theory/ Practical (Hrs/ Week)	Total No. of Hrs/ Semester	Duration of Exam. Hours	Max. Marks (Exam)	Continuous Evaluation	Total Marks	Credits
Ch-401 IC/PC	Solid State Chemistry	4	52	3	70	30	100	4
Ch-402 IC	Organometalic Chemistry & Catalysis	4	52	3	70	30	100	4
Ch-403 IC	Chemistry of Materials	4	52	3	70	30	100	4
Ch-404 IC/PC	Inorganic Spectroscopy	4	52	3	70	30	100	4
Ch-405	Inorganic Quantitative Analysis-I	4	60	4	35	15	50	2
Ch-406	Inorganic Quantitative Analysis-II	4	60	4	35	15	50	2
Ch-407	Instrumental Methods	4	60	4	35	15	50	2
Ch-408	Instrumental Methods	4	60	4	35	15	50	2
							600	24

**Scheme for continuous evaluation**

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IA : 15 Marks (based on Test + Seminar)

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**M. Sc. Chemistry (Organic Specialisation)  
III Semester**

Code No	Title	Theory/ Practical (Hrs/ Week)	Total No.of Hrs/ Semester	Duration of Exam. Hours	Max. Marks (Exam)	Continuous Evaluation	Total Marks	Credits
Ch-301 OC	Organic Reaction Mechanisms	4	52	3	70	30	100	4
Ch-302 OC	Organic Synthesis	4	52	3	70	30	100	4
Ch-303 IC/OC/PC	Organic Spectroscopy	4	52	3	70	30	100	4
Ch-304 OE	Open Elective	4	52	3	70	30	100	4
Ch-305	Practical-I Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-306	Practical-II Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-307	Practical-III Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-308	Practical-IV Inorg/Org/Phy	4	60	4	35	15	50	2
							600	24

**Scheme for continuous evaluation**

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**M. Sc. Chemistry (Organic Specialisation)**  
**IV Semester**

Code No	Title	Theory/ Practical (Hrs/ Week)	Total No.of Hrs/ Semester	Duration of Exam. Hours	Max. Marks (Exam)	Continuous Evaluation	Total Marks	Credits
Ch-401 OC	Stereochemistry and retrosynthetic analysis	4	52	3	70	30	100	4
Ch-402 OC	Chemistry of Natural Products	4	52	3	70	30	100	4
Ch-403 OC	Industrial Organic Chemistry	4	52	3	70	30	100	4
Ch-404 OC	Medicinal Organic Chemistry	4	52	3	70	30	100	4
Ch-405 OC	Preparation of Industrial Importance	4	60	4	35	15	50	2
Ch-406 OC	Extraction and Separations	4	60	4	35	15	50	2
Ch-407 OC	Instrumental Methods and Quantitative Analysis	4	60	4	35	15	50	2
Ch-408 OC	Qualitative Analysis of binary mixtures	4	60	4	35	15	50	2
							600	24

**Scheme for continuous evaluation**

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IA : 15 Marks (based on Test + Seminar)

  
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**M. Sc. Chemistry (Physical Specialisation)  
III Semester**

Code No	Title	Theory/ Practical (Hrs/ Week)	Total No.of Hrs/ Semest er	Duration of Exam. Hours	Max. Marks (Exam)	Continuous Evaluation	Total Marks	Credi ts
Ch-301PC	Applied Electrochemistry	4	52	3	70	30	100	4
Ch-302 PC	Quantum Chemistry and surface Chemistry	4	52	3	70	30	100	4
Ch-303 IC/OC/PC	Organic Spectroscopy	4	52	3	70	30	100	4
Ch-304 OE	Open Elective	4	52	3	70	30	100	4
Ch-305	Practical-I Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-306	Practical-II Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-307	Practical-III Inorg/Org/Phy	4	60	4	35	15	50	2
Ch-308	Practical-IV Inorg/Org/Phy	4	60	4	35	15	50	2
							600	24

**Scheme for continuous evaluation**

**A. Theory (each paper)**

Tests\* :30 Marks

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## M. Sc. Chemistry (Physical Specialisation)

### IV Semester

Code No	Title	Theory/ Practical (Hrs/ Week)	Total No. of Hrs/ Semester	Duration of Exam. Hours	Max. Marks (Exam)	Continu- ous Evaluati- on	Total Marks	Credits
Ch-401 IC/PC	Solid State Chemistry	4	52	3	70	30	100	4
Ch-402PC	Chemistry of Macromolecules and advanced photochemistry	4	52	3	70	30	100	4
Ch-403PC	Reaction Kinetics and Mechanisms	4	52	3	70	30	100	4
Ch-404 IC/PC	Inorganic Spectroscopy	4	52	3	70	30	100	4
Ch-405PC	Kinetics and Thermodynamics	4	60	4	35	15	50	2
Ch-406PC	Conductometric and potentiometric Experiments	4	60	4	35	15	50	2
Ch-407PC	Kinetics and Instrumental methods	4	60	4	35	15	50	2
Ch-408PC	Electrochemical and Instrumental methods	4	60	4	35	15	50	2
							600	24

#### Scheme for continuous evaluation

##### A. Theory (each paper)

Tests\* :30 Marks

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## QUESTION PAPER PATTERN

Semester I/II/III/IV

Sub: Chemistry

Time: 3 Hrs

Max. Marks: 70

Note: Answer question Number one and any **FIVE** in the remaining.

1. Answer any **TEN** sub divisions from the following (10x2=20)

a)  
b)  
c)  
d)  
e)  
f)  
g)  
h)  
i)  
j)  
k)  
l)

2 to 8

(a, b, or a,b,c)

(5x10=50)

(5+5) or (6+4) or (4+3+3)

2. Questions should be drawn from Unit-I
3. Questions should be drawn from Unit- II
4. Questions should be drawn from Unit- III
5. Questions should be drawn from Unit- IV

6, 7, 8 Questions should be drawn from Unit-I, II, III and IV.

  
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## SEMESTER – I

### Ch-101: INORGANIC CHEMISTRY- I

52h

#### UNIT- I

13h

**Chemical Bonding-** VSEPR model, shapes of molecules- $\text{ClF}_3$ ,  $\text{ICl}_4^-$ ,  $\text{TeF}_5^-$ ,  $\text{I}_3^-$ ,  $\text{TeCl}_6^{2-}$ ,  $\text{XeF}_6$ ,  $\text{SbCl}_6^{3-}$ ,  $\text{IF}_7$ ,  $\text{ReF}_7$ ,  $\text{XeF}_8^{2-}$ ,  $\text{TaF}_8^{3-}$ ; Bent rules and energetics of hybridization; electronegativity-Pauling, Allred-Rochow and Mulliken, electronegativity and partial ionic character; Bonds-Multicenter, Synergic and Agostic bonding. Lattice energy: Born-Lande equation, Kapustinskii equation; Fajan's rules- polarizability and partial covalent character, radius-ratio rules-limiting radius ratios of trigonal, tetrahedral, octahedral and cubic. Structures of solids- $\text{NaCl}$ ,  $\text{CsCl}$ ,  $\text{ZnS}$  (zinc blende and wurtzite), rutile( $\text{TiO}_2$ ), perovskite( $\text{CaTiO}_3$ ), fluorite and anti fluorite. Zintl ions, Molecular orbital theory: formation of sigma, pi and delta bonds, LCAO and MO diagrams of heteronuclear diatomic ( $\text{CO}$ ,  $\text{NO}$ ,  $\text{HF}$  and  $\text{ICl}$ ) and triatomic molecules ( $\text{CO}_2$  and  $\text{NO}_2$ ).

#### UNIT- II

13h

**Chemistry of main group elements:-** Boranes- nomenclature, synthesis, structure and bonding in boranes, styx code, carboranes- classification, structures of ortho, meta, para- $\text{C}_2\text{B}_{10}\text{H}_{12}$ , Wades rules, Metallocarboranes- synthesis and structure of  $[\text{Fe}(\eta^5\text{-C}_2\text{B}_9\text{H}_{11})_2]^{2-}$ ,  $\text{Fe}(\eta^5\text{-C}_2\text{B}_9\text{H}_{11})(\eta^5\text{-C}_5\text{H}_5)$ ,  $[\text{Mo}(\text{CO})_3(\eta^5\text{-C}_2\text{B}_9\text{H}_{11})]^{2-}$ , synthesis, structure and bonding in borazine, phosphazenes- synthesis, structure and bonding in  $(\text{PNCl}_2)_3$ , S,N- compounds-  $\text{S}_4\text{N}_4$ ,  $\text{S}_2\text{N}_2$  and polythiazyl.

**Silicates:-** Principles of silicates structures, classification with examples-ortho, pyro, cyclo, ino, phyllo and tecto silicates, isomorphous replacement; zeolites- sodalite and pentasil units, synthesis and structures of ZSM-5, zeolite A, faujasite and their uses.

#### UNIT-III

13h

**HSAB concept:** Basis of HSAB concept, acid-base strength, hardness and softness, symbiosis, applications and limitations of HSAB concept; Acid- base concept in non-aqueous media, reactions in  $\text{BrF}_3$ ,  $\text{N}_2\text{O}_4$ , anhydrous  $\text{H}_2\text{SO}_4$ ,  $\text{CH}_3\text{CO}_2\text{H}$ . Isopoly and heteropoly acids of W and Mo, preparations, properties, structure and applications.

**Stereoisomerism:-** Chirality, optical activity- CD, ORD, Cotton effect, absolute configuration of metal complexes, magnetic circular dichroism and its uses.

#### UNIT-IV

13h

**Metal clusters-** factors favouring M-M bond, classification, synthesis, structure and bonding in  $[\text{Re}_2\text{Cl}_8]^{2-}$ . Metal carbonyl clusters- LNCC's and HNCC's. Electron counting in carbonyl clusters, Wades-Mingos and Lauher rules.

**Nuclear Chemistry-**The atomic nucleus-elementary particles, quarks, classification of nuclides based on Z and N values, nuclear stability, nuclear potential, binding energy. Nuclear

Models: Shell model-salient features, forms of the nuclear potential, filling of orbitals, nuclear configuration, Liquid drop model. Radioactivity, radioactive decay kinetics, Parent-daughter decay-growth relationship-secular and transient equilibria, theories of  $\alpha$ ,  $\beta^-$ ,  $\beta^+$  and  $\gamma$ -decay, internal conversion, Auger effect.

### SUGGESTED BOOKS

1. Basic Inorganic Chemistry- F. A. Cotton, G. Wilkinson and P. L. Gaus; John Wiley and sons. Inc, 3<sup>rd</sup> edition (2004).
2. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson. 6<sup>th</sup> edition (1999).
3. Inorganic Chemistry, J. E. Huheey, E. A. Keiter and R. L. Keiter, IV edition Addison; Wesley (1993).
4. Inorganic Chemistry, D. F. Shriver, P. W. Atkins and C. H. Langford, V edition ELBS; Oxford University Press, (2010)
5. Chemistry of elements; N. N. Greenwood and A. E. Earnshaw, Butterworth, II edition Heinemann (1997).
6. Concise Inorganic Chemistry, J. D. Lee , 5th edition; (1996).
7. Essentials of nuclear chemistry, H. J. Arniker, 4<sup>th</sup> edition; NAIL publishers (2011) Chapters 1, 3 and 4.
8. Nuclear and Radio chemistry; G.Friedlander, J.W.Kennedy, ES Macias and JM Miller; 1981, Chapters 8and 9.
9. Inorganic Chemistry, Gary. L. Miessler and Donald . A. Tarr 5<sup>th</sup> Edition; (2014).
10. Inorganic Chemistry CE House croft and A G Sharpe 4<sup>th</sup> edition, pearson (2012).

## Ch-102: ORGANIC CHEMISTRY- I

52h

### UNIT-I

#### **Nature of Bonding in Organic Molecules**

13h

*Delocalized chemical bonding:* Conjugation, cross conjugation, resonance. Hyperconjugation. Tautomerism.

*Aromaticity:* Huckel's MO theory. HMO diagram for benzene. Huckel's rules of aromaticity. Aromatic systems with electron numbers other than six (including azulene, tropone, tropolone and annulenes). Anti-aromaticity. Aromaticity in benzenoids. Homo-aromaticity. Alternant and non-alternant hydrocarbons. Energy levels in odd and even-alternant hydrocarbons, energy levels for the benzyl cation, benzyl free-radical and benzyl carbanion.

Mesoionic compounds. Heteroannulenes. Fullerenes: C-60.

*Synthetic Molecular Receptors:* Definition and significance. Structure and function of receptors with molecular clefts, molecular tweezers, receptors with multiple hydrogen bonding sites. Crown ethers, cryptates, cyclodextrins, cyclophanes, catenanes and rotoxanes, calixarenes, ionophores and micelles.

## UNIT-II

### **Reaction Mechanisms:**

13h

*Reactive intermediates:* Generation, structure, stability and reactivity of carbocations, carbanions, carbon free radicals, carbenes. Non-classical carbocations, nitrenes.

Reactions and mechanisms: Thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates.

Methods of determining mechanisms: Based on the structure of products, determination of the presence of intermediates, isotopic labeling, isotope effects, from stereochemical evidence.

*Acids and bases:* Hard and soft acids and bases. Effect of structure on the strengths of acids and bases.

*Effect of structure on reactivity:* Resonance and field effects; steric effects. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

*Aliphatic substitution reactions:*

*Nucleophilic substitution reaction at a saturated carbon:*  $S_N1$ ,  $S_N2$ , and SET mechanisms. Effect of substrate structure, attacking nucleophile and leaving group. Neighbouring group participation by sigma and pi bonds. Anchimeric effect. Ambident nucleophiles and substrates.

*Electrophilic substitution reaction at a saturated carbon:*  $S_E1$ ,  $S_E2$ , and  $S_{Ei}$  mechanisms. Effect of substrate structure, leaving group and solvent polarity on the reactivity.

## UNIT-III

### **Stereochemistry**

13h

***Projection formulae: Fischer, Newman, Sawhorse and flying wedge projections - their interconversions for acyclic and cyclic compounds.***

*Conformational analysis:* D/L, R/S and M/P conventions. Cahn-Ingold Prelog (CIP) sequence rules.

Optical isomerism: Elements of symmetry and chirality. Chirality in compounds with a stereogenic centre. Center of chirality, axis of chirality, plane of chirality and helicity. Stereochemistry of allenes, alkylidene cycloalkanes and spiranes (with a stereogenic axis), biphenyls, cyclophanes, ansa compounds, *trans*-cyclooctene, helicenes, benzphenanthrenes. Configurational nomenclature.

*Conformational analysis:* Conformational analysis of cycloalkanes: cyclobutane, cyclopentane, cyclohexanes (mono-substituted e.g., methyl, *iso*-propyl, *tert*-butyl and di-substituted cyclohexanes e.g., dialkyl-, dihalo-, diols), and cycloheptane.

Nomenclature and conformations of fused rings and bridged ring systems.

*Prochirality:* Enantiotopic and diastereotopic atoms, groups and faces. [Si/Re]. Basics of Cram's and Prelog's rules of asymmetric induction.

## UNIT-IV

### **Carbohydrates:**

13h

Introduction. Determination of configuration of the mono saccharides, conformational analysis of monosaccharides. Synthesis of aldonic, uronic, aldaric acids and alditols. Derivatives of monosaccharides: acetals, ethers, aminosugars and deoxysugars. Structural elucidation of sucrose and maltose. Structures of lactose, gentiobiose and meliobiose. Photosynthesis of carbohydrates.

## Heterocyclic compounds:

Introduction. Nomenclature of simple and fused heterocyclic compounds. Synthesis and reactions of pyrazole, imidazole, oxazole, isoxazole, thiazole and isothiazole. Synthesis of benzimidazole, benzoxazole, benzisoxazole, indole and coumarins.

## Vitamins

Introduction. Biological importance and synthesis of Vitamin A, Vitamin B<sub>1</sub> (thiamine), Vitamin B<sub>6</sub> (pyridoxine), folic acid, pantothenic acid, riboflavin, Vitamin C, Vitamin E ( $\alpha$ -tocopherol), Vitamin H (biotin), Vitamin K<sub>1</sub> and K<sub>2</sub>.

## SUGGESTED BOOKS

1. Organic Chemistry, R T Morrison, R N Boyd and S K Bhattacharjee, 7th edition, Pearson, (2018).
2. Organic Chemistry, J Clayden, N Greeves and S Warren, 2<sup>nd</sup> edition, Oxford University Press, (2014)
3. Advanced Organic Chemistry – Reactions, Mechanism and Structure, J March, John Wiley (2008).
4. Advanced Organic Chemistry, F A Carey and R J Sundberg Plenum, (2000).
5. A Guide Book to Mechanism in Organic Chemistry, P Sykes, 6th edition, Pearson, (2003).
6. Structure and mechanism of Organic Chemistry, C K Ingold, 2nd Edition, CBS, (2016).
7. Principles of Organic Synthesis, 3rd edition, R O C Norman and J M Coxon, Blackie Academic and Professional (Indian Reprint), (2012).
8. Stereochemistry, V R Dani, Asian Books, New Delhi, (2014).
9. Stereochemistry of Organic Compounds, D Nasipuri, 3rd edition, New-Age International, (2018).
10. Organic Stereochemistry, M J T Robinson, Oxford University Press, (2005).
11. Stereochemistry of Carbon Compounds, E L Eliel, S H Wilen and L N Mander, John Wiley, (1994).
12. Stereochemistry at a Glance J Eames, J M Peach, Blackwell, Oxford, (2003).
13. Heterocyclic Chemistry at a Glance, II edition, J A Joule and K Mills, Wiley, New York, (2012).
14. Organic Chemistry, Volume I, I L Finar, 6th edition, Pearson, (2018).
15. Organic Chemistry, Volume II, I L Finar, 6th edition, Pearson, (2018)

**UNIT-I****Quantum Mechanics-I      13h**

Introduction to quantum mechanics. Schrödinger wave equation. Time-independent and time dependent Schrödinger wave equations and the relation between their solutions. Eigen functions and Eigenvalues. Physical Interpretation of wave function. Concepts of Operators: Laplacian, Hamiltonian, Linear and Hermitian operators. Angular Momentum operators and their properties. Commutation of operators. Normalization, orthogonality and orthonormality of wave functions. Average (expectation) values. Postulates of quantum mechanics. Solutions of Schrödinger wave equation for a free particle, particle in a ring, particle in a three dimensional box. Quantum mechanical degeneracy, tunneling (no derivation). Application of Schrödinger equation to harmonic oscillator, rigid rotator. Eigen functions and eigenvalues of angular momentum. Ladder operator method for angular momentum.

**UNIT-II****Quantum Mechanics-II      13h**

Schrödinger equation to hydrogen atom in spherical polar co-ordinates. Solution of equation and statements of solution of R equation. Total wave functions of hydrogen atom. Quantum numbers and their characteristics. List of wave functions for few initial states of hydrogen like atoms. Diagrams of radial and angular wave functions. Radial and angular distribution function and their significance. Electron spin

(Stern-Gerlach experiment), spinorbital, anti symmetry and Pauli-exclusion principle, Slater determinants. Coupling of Angular momenta. Russell-Saunders and JJ-coupling, Atomic Term symbols. Spin-orbital interaction and explanation of term multiplicities (Na-D doublet). Zeeman effect.

Approximate methods: Need for approximate methods. Perturbation method. Rayleigh Schrödinger perturbation theory for time-independent non-degenerate system. Application to electron in a box under the influence of an electric field. Application to He atom. Variation theory-statement and proof. Application of variation method to particle in a one-dimensional box and He atom.

**UNIT-III****Chemical Dynamics-I****13hr**

Macroscopic and microscopic kinetics, Review of theories of reaction rate-Collision theory and Transition state theory, Comparison of collision theory with transition state theory, Arrhenius equation- characteristics, Significance of energy of activation, Temperature coefficient and its evaluation. Thermodynamical formulation of reaction rates (Wyne-jones and Eyring treatment), Reaction between ions in solutions – Influence of ionic strength on reaction rates (primary and secondary salt effects).

Concept of Steady state kinetics, Chain reactions – chain length and chain inhibition, comparison of photochemical and thermal reactions, Mechanisms of thermal and photochemical

reactions between hydrogen-bromine and hydrogen-chlorine. Comparative study of thermal and photochemical hydrogen-halogen reactions. Pyrolysis of acetaldehyde, Decomposition of ethane.

Kinetics of fast reactions- Introduction, Study of reactions by relaxation method (Temperature and pressure jump), flow method (Plug flow method and Stopped flow method), Flash photolysis and Shock tube method.

#### UNIT-IV

##### **Chemical Dynamics-II**

13hr

Kinetics of homogeneous catalysis: kinetics of auto catalytic reactions, kinetics of acid-base catalysed reactions. Comparison of enzyme catalysed and chemical catalysed reactions, Mechanism (Lock and Key theory), Kinetics of enzyme catalyzed reactions – Henri-Michaelis-Menten mechanism, Significance of Michaelis-Menten constant, Lineweaver-Burk plot. Effects of enzyme concentration, pH, Temperature, Activators and Inhibitors on enzyme activity.

Unimolecular reactions: Perrin theory, Lindemann theory, and Hinshelwood theory.

Surface chemistry: Types of adsorption isotherms, Effect of temperature on adsorption, Mechanical adsorption, Estimation of surface area using BET equation, Gibbs adsorption isotherm and its significance, Surface tension and surface energy, Pressure difference across curved surface (Laplace equation), Vapour pressure of droplets (Kelvin equation), Surface film on liquids (electro-kinetic phenomena), Catalytic activity of surfaces.

#### **SUGGESTED BOOKS**

1. Physical Chemistry- P. Atkins and J. D. Paula, 9th Edn., Oxford University Press (2010).
2. Physical Chemistry: A Molecular Approach, D. A. McQuarrie and Simon, Viva, New Delhi, (2003).
3. Introduction to Quantum Chemistry, A. K. Chandra, 3<sup>rd</sup> Edn. Tata McGraw Hill, (1991).
4. Quantum Chemistry, Ira. N. Levine, Prentice Hall, New Jersey, (1991).
5. Quantum Chemistry, R. K. Prasad, New Age International, 4<sup>th</sup> Edn., (2010).
6. Quantum Mechanics by G R Chatwal and S K Anand, Himalaya Publications, 8<sup>th</sup> Edn, 2012.
7. Chemical Kinetics- K. J. Laidler, McGraw Hill. Inc. New York (1988).
8. Principles of Chemical Kinetics – House J. E. Wm C Brown Publisher, Boston, (1997).
9. Kinetics and Mechanism of Chemical Transformations- J. Rajaraman and J. Kuriakose, Mc Millan India Ltd. (2011).
10. Biochemistry, - Geoffrey Zubay, 2nd Edn., Macmillan Publishing Co. New York (1988).
11. Physical Chemistry of Surfaces- A. W. Adamson, Wiley-Interscience Publisher Inc., New York (1997).
12. Introduction to surface chemistry and Catalysis by Gabor A. Somorjai and Yimin Li, John 2<sup>nd</sup> Edn. Wiley and Sons Ltd, Hoboken, United States, 2010.

## Ch-104 : ANALYTICAL CHEMISTRY

### UNIT – I

#### **Basic concepts**

13 h

Safety measures in chemical laboratories, Fire hazards, toxic chemicals: Acids/bases/solvents handling, storage, dilution, disposal of chemicals, acid/ solvent bottles etc. toxic chemicals sampling and handling hazards, safety data sheets, miniaturization of analytical instruments, their significance in modern chemical analysis.

Preparation of dilute acids from concentrated/fuming acids like  $\text{H}_2\text{SO}_4$ , handling liquid bromine, elemental mercury, solvent ether, liquor ammonia, liquid nitrogen.

**Errors in chemical analysis:** absolute, relative error, random error distribution, Gaussian curve, Limitations of analytical methods, determinate and indeterminate errors, minimization of errors. Accuracy and precision, distribution of random errors, the normal error curve. Statistical treatment of finite samples - measures of central tendency and variability: mean, median, range, standard deviation, variance, confidence limits, Comparison of an experimental mean and a true mean. F-test, rejection of result - Q-test, Student's t-test, numerical problems.

### UNIT-II

#### **Quantitative Analysis-Classical methods**

13 h

Classification of analytical methods, types of instrumental analysis, factors influencing choice of analytical method, qualitative and quantitative analysis, Units used in chemical analysis, their conversion, ppm, ppb, ppt etc.

#### **Titrimetry**

**Acid-Base:** Theory of indicators, Ex: Phenolphthalein, Methyl red. Titration curves for mono functional acid and base, pH calculations, fractions of phosphoric acid species as a function of pH. Titration curves for  $\text{H}_3\text{PO}_4$ .

**Complexometry:** Theory of metal ion indicators, EDTA titrations, suitability of polydentate ligands as titrants, expressions for the different forms of EDTA in solution as a function of pH, conditional stability constants, effect of pH and nature of titration curve. Masking and demasking, type of EDTA titrations, titrations involving monodentate, bidentate and polydentate ligands.

**Redox:** Mechanism of indicator action, criteria for the selection of indicators. Feasibility of redox titration. Titration of multicomponent system. Nernst equation. Applications: Oxidants such as Ce(IV), bromate, Iodates.

**Precipitation:** Solubility product. Theoretical principles of precipitation: Titration curve, end point detection, Mohr, Volhard and adsorption indicators. Applications: Estimation of  $\text{F}^-$ ,  $\text{K}^+$ ,  $\text{CO}_3^{2-}$ ,  $\text{C}_2\text{O}_4^{2-}$ , acetylenes and mixture of halides.

#### **Gravimetry**

Quantitative precipitation, *Precipitation from Homogeneous Solution (PFHS)*, Formation and treatment of precipitates, co-precipitation, post precipitation. Conditions for precipitation, washing, drying and igniting the precipitates, Important precipitating agents such as DMG, oxine, thiocyanate and their significance in inorganic analysis. errors in gravimetric analysis.

### Unit-III

13h

#### **Quantitative Analysis – Instrumental methods**

Electromagnetic radiation, interaction with matter, absorption, Beer-Lambert's law, derivation, molar absorptivity, Sandell sensitivity, Ringbom plot, deviations, limitations, Calibration with standards, standard addition, internal standard addition, limit of detection, limit of quantification, Instrumentation, radiation sources, wavelength selection devices, optical slits, single beam and double beam instruments, photo electric colorimeter, scanning devices, merits and limitations, numerical problems on application of Beer's law.

### Unit IV

13h

#### **Separation Methods**

Solvent Extraction – Types ,batch, continuous, efficiency, selectivity. Distribution coefficient, Nernst distribution law, derivation, factors affecting the partition, applications. Chromatography – Types, Terminology, Principles of paper, thin layer, column, gas chromatography, column efficiency, plate theory, factors affecting the column efficiency, band broadening,  $R_f$  factor, Van-Deemter equation, medium performance liquid chromatography, high performance liquid chromatography, reserved phase liquid chromatography, super critical fluid chromatography, characteristics of super critical fluids, 2D-thin layer chromatography, electrophoresis, principles, applications etc. numerical problems on solvent extraction,  $R_f$  factor and van Demeter equation.

#### **SUGGESTED BOOKS:**

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch, 8<sup>th</sup> edition, Saunders College Publishing, New York, 2005.
2. Analytical Chemistry, G.D. Christian, 6<sup>th</sup> edition, John Wiley & Sons, Inc, India, 2004.
3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6<sup>th</sup> edition, Prentice Hall, Inc. New Delhi, 1993
4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6<sup>th</sup> edition, Third Indian Reprint, Pearson Education Pvt. Ltd., New Delhi, 2003.
5. Analytical Chemistry Principles, John H. Kennedy, 2<sup>nd</sup> edition, Saunders College Publishing, California, 1990.
6. Principles and Practice of Analytical Chemistry, F.W. Fifield and Kealey, 3<sup>rd</sup> edition, Blackwell Sci., Ltd. Malden, USA, 2000.
7. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.
8. Practical Volumetric Analysis, Peter A C McPherson, RSC, Cambridge, UK, 2015.
9. Analytical Chemistry for Technicians, John Kenkel, 4<sup>th</sup> edn. CRC Press, London, 2014.
10. Undergraduate Instrumental Analysis, J.W. Robinson, E.M. Skelly Frame, G. M. Frame II, 6<sup>th</sup> edn. Marcel Dekker, New York, 2009.

## Ch-105: MATHEMATICS FOR CHEMISTS

### UNIT-I

12h

**Vectors:** vectors, dot and cross products; scalar and vector triple products and their applications. Tensors and their applications.

**Matrix Algebra:** Review of different types of matrices (including Hermetian and skew Hermetian); matrix addition and multiplication; determinant of a square matrix, transpose, adjoint and inverse of a square matrix. Solution to system of linear equation (a) by matrix method and (b) by Cramer's Rule. Characteristic equation of a square matrix, eigenvalues and eigenvectors.

### UNIT-II

12h

**Calculus:** Rule for differentiation; Chainrule (for  $f(x)=U^n$ ,  $\sin u$ ,  $\log u$  etc). Implicit differentiation and parametric differentiation and successive differentiation of order 2 (for explicit functions only).

Applications of differentiation: Derivative as a slope of the tangent, derivative as a rate measure-velocity and acceleration. Increasing and decreasing functions-Maxima and minima-second derivative test-point of inflections-problems restricted to polynomial.

### UNIT-III

12h

**Integrations:** Basic rules-simple substitution-Method of partial fractions-Integration by parts. Define integral and application to areas of plane curves.

Functions of several variables: partial derivatives; co-ordinate transformation from cartesian co-ordinates to spherical and cylindrical coordinates and vice-versa.

**Elementary differential equation:** Variable separable, exact first order equations, linear and homogeneous equation.

Second order homogeneous differential equation with constant coefficients  $f(D)$ ,  $y=0$ . Solution of differential equation by power series method.

Fourier series: Simple problems.

**Probability:** Review of permutations and combinations. Probability and addition theorem for mutually exclusive events and multiplication theorem for independent events. Curve fitting-Method of least squares.

### **SUGGESTED BOOKS**

1. Mathematical Preparation for physical chemistry, F. Daniells, M.Graw Hill Inc., US, 1959.
2. Mathematics for chemists, D. M. Hirst, Chemical Publishing Company Incorporated, New York, 1979.
3. Mathematics for chemists, P. G. Francis, Springer, 2011.
4. Basic Mathematics for chemists, P. Tebutt, Wiley-Blackwell, 1994.
5. Calculus and analytic geometry, 9<sup>th</sup> edition, G. B. Thomas, R.L. Finney, Addison-Wesley Publishing Company, Inc. 1996.
6. Short Course in differential equations, Rainvilles and Bedient, IBH publishers, 1968.

7. Mathematics for chemistry, G. Doggett and B. T. Sutcliffe Longmann Publishers, 1995.

## INORGANIC CHEMISTRY PRACTICALS

(4 days a week, 4 hours a day)

### C-106 : Inorganic Practical-I (Semi-micro Qualitative Analysis)

Semi micro qualitative analysis of mixtures containing two anions, two common cations and one less familiar elements: W, Mo, Ce, Zr, V and Li.

### C-107: Inorganic practical-II (Complex preparation)

Preparation of inorganic complexes:

1. Cis- potassium dioxalatodiaquachromium(III) complex.
2. Hexamminecobalt(III) chloride.
3. Mercury tetrathiocyanatocobaltate.
4. Pentamminechlorocobalt(III) chloride.
5. Potassium tris(oxalato)ferrate trihydrate.
6. Potassium tris(oxalato)aluminate trihydrate.

### C-108: Inorganic Practical-III (Gravimetry)

#### Gravimetric analysis

1. Determination of Fe in iron ore as  $\text{Fe}_2\text{O}_3$ .
2. Determination of Ni as nickel dimethylglyoximate in Cu and Ni solution.
3. Determination of Ca as  $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ .
4. Determination of Al as aluminiumoxinate.
5. Determination of Cu as  $\text{CuSCN}$  in Cu and Fe solution.
6. Determination of Zn as  $\text{ZnNH}_4\text{PO}_4$ .

### C-109 :Inorganic Practical-IV (Volumetry)

#### Volumetric analysis

1. Determination of Ca and Mg in Dolomite solution using EDTA.
2. Determination of Cu in Cu and Ni solution iodometrically.
3. Determination of Fe in Cu and Fe solution (using  $\text{K}_2\text{Cr}_2\text{O}_7$ ).
4. Determination of Cr and Fe in a mixture using ceric ammoniumsulphate.
5. Determination of Fe and Al in mixture using EDTA.
6. Determination of percentage of Fe and oxalate in  $\text{K}_3\text{Fe}(\text{C}_2\text{O}_4)_3 \cdot 3\text{H}_2\text{O}$

### SUGGESTED BOOKS

1. Vogel's Text book of Qualitative Chemical Analysis, J. Bassett, G. H. Jeffery and J. Mendham, 7<sup>th</sup> edition, ELBS (2013).
2. Vogel's text book of Quantitative Chemical Analysis, 6<sup>th</sup> Edition, J. Bassett, G. H. Jeffery and J. Mendham, and R. C. Denny, J D Barnes, M.Thomas Prentice Hall (2000)
3. Inorganic Semimicro Qualitative Analysis, V. V. Ramanujam; The National Pub. Co. (1990).
4. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Von Nostrand Reinhold Co.,

London (1972).

5. An Advance course in practical chemistry, A Ghoshal, B Mahapatra and A K Nad; New central book agency Pvt.Ltd. 3<sup>rd</sup> edition 2007.
6. Advanced inorganic analysis, S K Agarwal and Keemtilal; Pragati prakashan, 12<sup>th</sup> edition 2014.

## ORGANIC CHEMISTRY PRACTICALS

(4 days a week, 4 hours a day)

### Ch-106 : Organic Practical-I (Preparation –One stage)

#### Preparation (one stage)

1. Oxidation of cyclohexanol.
2. Preparation of S-benzylisothiuroniumchloride.
3. Synthesis of picric acid.
4. Synthesis of glucose pentaacetate.
5. Synthesis of 2,4,6-tribromoaniline.
6. Cannizarro reaction: benzaldehyde to benzyl alcohol and benzoic acid.
7. Dehydration of cyclohexanol to cyclohexene.
8. Claisen-Schmidt reaction: benzaldehyde and acetone to dibenzalacetone.
9. Sandmeyer reaction: 4-chlorotoluene from 4-toluidine.
10. Pechmann reaction: resorcinol and ethylacetoacetate to 7-hydroxy-4-methylcoumarin
11. Synthesis of 2,4-dichlorophenoxyacetic acid.
12. Synthesis of resacetophenone .

### Ch-107: Organic Practical-II (Qualitative Analysis)

Qualitative analysis: Systematic analysis and identification of bifunctional organic compounds.

### Ch-108 :Organic Practical – III (Preparation two/ three stages)

1. 4-Bromoaniline from acetanilide.
2. 3-Nitrobenzoic acid from benzoic acid/methyl benzoate.
3. 2,4-Dinitrophenylhydrazine from chlorobenzene.
4. N-Methylantranilic acid from phthalic acid.
5. Benzanilide from benzophenone.
6. Benzilic acid from benzoin.
7. Synthesis of acridone.
8. Synthesis of hydantoin.
9. Anthracene to anthrone
10. Succinic acid to N-bromosuccinimide.
11. Maleic acid to dimethylacetylenedicarboxylate.

### Ch-109 : Organic Practical-IV (Quantitative Analysis)

Quantitative analysis

1. Titrimetric estimation of mono-, dicarboxylic-, amino- and aryloxyacetic acids.

2. Saponification value of oil.
3. Estimation of glucose by Fehling's method/Bertrand's method.
4. Estimation of keto-group.
5. Estimation of phenols.
6. Iodine value of oil (Chloramine-T method)
7. Acid and ester, acid and amide in the mixture of two.

### SUGGESTED BOOKS

1. Vogel's Text Book of Practical Organic Chemistry – 5th edition, B. S. Furniss, A. J. Hannaford, P. W. G. Smith and A. R. Tatchell - Pearson, (2003).
2. Laboratory manual of Organic Chemistry- B. B. Dey, M. V. Sitaraman and T.R. Govindachari, Allied Publishers, New Delhi, (1996).
3. Practical Organic Chemistry, IV edition, – F. G. Mann and B. C. Saunders, - Pearson, 2009).
4. Text Book of Practical Organic Chemistry including qualitative analysis – IV Edition, A. I. Vogel and A. R. Tatchell, Longman, London, (1996).
5. Test Book of Quantitative Organic Analysis- A. I. Vogel, (1996).
6. A Handbook of Organic Analysis – Qualitative and Quantitative – IV Edition, H. T. Clarke, Hodder and Staughton, New Delhi (2017).
7. Comprehensive practical organic chemistry: Preparation and quantitative Analysis, V. K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000.
8. Comprehensive practical organic chemistry: Qualitative analysis, V. K. Ahluwalia, S. Dhingra, Universities Press (India), 2000.
9. An advanced course in practical chemistry, A. Ghoshal, B. Mahapatra and A.Kr. Nad, New central book agency, Calcutta, 2000.
10. Advanced practical organic chemistry, J. Mohan, Vol. I and II, Himalaya Publishing House, 1992.
11. Practical organic chemistry (Quantitative analysis), B. B. Dey, M. V. Sitaraman and T. R. Govindachari, Allied Publishers, New Delhi, 1992.
12. Advanced Practical Organic Chemistry, III Edition, J. Leonard, B. Lygo and G. Procter, CRC Press, Routledge, (2013).
13. Qualitative Organic Analysis – Spectrochemical Techniques W. Kemp, II edition, Mc-Graw Hill, London, (1986).

### PHYSICAL CHEMISTRY PRACTICALS (4 days a week, 4 hours a day)

#### C-106 : Physical Chemistry Practical -I

1. Study of Acid catalysed hydrolysis of methyl acetate at lab temperature and reporting the calculated and graphical rate constants
2. Determination of Velocity constant for the saponification of Ethyl acetate at lab temperature and comparing it with graphical value.
3. Verification of Beer's Law: Colorimetric estimation of  $\text{Cu}^{2+}$  ions and reporting the Molar extinction coefficient.
4. Determination of heat of solution of a sparingly soluble salt.
5. Colorimetric estimation of  $\text{Fe}^{2+}$  ions in a given solution by titrating FAS versus  $\text{KMnO}_4$  solution.
6. Study of kinetics of the reaction between KI and  $\text{K}_2\text{S}_2\text{O}_8$  solution.
7. Construction of phase diagram of two component systems and determination of  $E_c$ ,  $E_T$  and the

- Composition of given unknown.
- Determination of partial molar volume of solute – water system by apparent molar volume method.
  - Analysis of a binary mixture by viscosity measurement method.
  - Verification of Freundlich and Langmuir isotherm for adsorption of oxalic/acetic acid on activated charcoal.

### **C-107: Physical Practical -II**

#### **Conductometric Experiments**

- Precipitation titration of lithium sulphate versus  $\text{BaCl}_2$  and reporting the concentration of  $\text{Li}_2\text{SO}_4$ .
- Determination of concentration of a weak acid by titrating against a weak base.
- Determination of a dissociation constant of weak acid ( $\text{CH}_3\text{COOH}$ ).
- Determination of Equivalent conductance of a given strong electrolyte.
- Determination of the concentration of a strong acid and a salt in a given mixture of by titrating against a strong base.

#### **Potentiometric Experiments**

- Determination of single electrode potential of  $\text{Cu}^{2+}/\text{Cu}$  and estimate the given unknown concentration.
- Determination of single electrode potential of  $\text{Zn}^{2+}/\text{Zn}$  and estimate the given unknown concentration.
- Titration of  $\text{AgNO}_3$  versus  $\text{KCl}$  and estimation of the concentration of  $\text{AgNO}_3$ .
- Determination of  $\text{pK}_a$  and  $\text{K}_a$  values of the weak acid by titrating against a strong base using quinhydrone electrode.
- Determination and comparison of pH values of buffer solutions by using quinhydrone electrode and glass electrode.

### **C-108 : Physical Chemistry Practical -III**

- Study of acid hydrolysis of methyl acetate for two different concentrations of  $\text{HCl}$  and reporting the relative strength.
- Study the hydrolysis of methyl acetate in the presence of  $\text{HCl}$  at two different temperatures and reporting the energy of activation.
- Determination of dissociation constant of a given indicator by colorimetric method.
- Study of kinetics of autocatalytic reaction between  $\text{KMnO}_4$  versus oxalic acid.
- Determination of degree of hydrolysis of aniline hydrochloride at room temperature and calculation of dissociation constant of the base by pH metry.
- Study of variation of viscosity of a liquid with temperature and determination of the constants A and B.
- Analysis of a binary mixture of two miscible liquids by surface tension method
- Construction of phase diagram of Urea -  $\text{KCl}$  -  $\text{H}_2\text{O}$  system.
- Determination of heat of neutralization of two acids and their relative strength.
- Evaluation of Arrhenius parameter for the reaction between  $\text{K}_2\text{S}_2\text{O}_8$  versus  $\text{KI}$  (first order)

## C-109 : Physical Chemistry Practical -IV

### Conductometry

1. Determination of concentration of mixture of strong acid and weak acid versus strong base.
2. Determination of concentration of Weak acid with salt versus strong base.
3. Determination of strength of a strong acid, weak acid and a salt versus strong base  
pH metry
- 5 Determination of the acidic and basic dissociation constant and isoelectric point of an amino acid by  
pH metry.
6. Determination of pKa value or Dissociation constant of phosphoric acid.
7. Determination of pH of acetic acid with sodium acetate buffer.  
Potentiometry
8. Determination of concentration and amount of  $K_2Cr_2O_7$  by titrating against FAS and calculation of redox potential.
9. Determination of concentration of mixture of acids by titrating against NaOH solution.
10. Determination of concentration of  $KMnO_4$  by titrating against FAS and calculation of redox potential.

### SUGGETED BOOKS

1. Advanced Practical Physical Chemistry by J. B. Yadav, Goel Publications, Meerut (2012).
2. Senior Practical Physical Chemistry by B. C. Kosla, Simla Printers, New Delhi (1987).
3. Experimental Physical Chemistry by Daniel et al., McGraw Hill, New York (1962).
4. Practical Physical Chemistry by A.M James and P. E. Pritchard, Longman's Group Ltd (1968).
5. Experimental Physical Chemistry by Wilson, Newcombe & others, Pergamon Press, New York (1962).
6. Experimental Physical Chemistry by R. C. Behra and B Behra, Tata McGraw, New Delhi (1983).
7. Experimental Physical Chemistry by V. D. Atavale and Parul Mathur, New Age International, New York (2001).
8. Practical's in physical chemistry A. Modern Approach by P.S Sindhu, Mac. Millan Publishers, Delhi (2006).

## II SEMESTER

### Ch-201: INORGANIC CHEMISTRY- II

#### UNIT-I

13h

**Metal-Ligand equilibria in solution-** Step-wise and overall formation constant and their relationship, trends in step-wise constant, kinetic and thermodynamic stability of metal complexes, factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, chelate effect, macrocyclic effect and their thermodynamic origin. Determination of binary formation constant by pH metry, spectrophotometry, polarography and ion exchange methods.

**Structure and bonding-** hydride, dihydrogen, dioxygen, isocyanide, N<sub>2</sub> and tertiary phosphine complexes of transition metals, metal carbonyls-terminal and bridge carbonyls, detection, metal nitrosyls- terminal (linear and bent) and bridge.

#### UNIT-II

13h

**Metal- ligand bonding-** Coordination numbers 3 to 8. Crystal field theory, salient features, spectrochemical series, splitting of d-orbitals in tetrahedral, square planar, trigonal bipyramidal, square-pyramidal and octahedral geometry, applications of CFT- colors of transition metal complexes, magnetic properties of octahedral complex, Jahn Teller distortion, CFSE and their uses, factors affecting CFSE, limitations of CFT, experimental evidences for metal-ligand covalent bonding in complexes, nephelauxetic effect, Ligand Field Theory, MO theory: tetrahedral and octahedral complexes (including  $\pi$ -bonding), angular overlap model. Stereochemical non-rigidity and its detection.

#### UNIT-III

**Electronic spectra of coordination compounds-** Spectroscopic ground states, selection rules, term symbols for d<sup>n</sup> ions, Racah parameters, Orgel, Correlation and Tanabe-Sugano diagrams, spectra of 3d metal-aqua complexes of trivalent V, Cr, divalent Mn, Co and Ni, CoCl<sub>4</sub><sup>2-</sup>, calculation of Dq, B and  $\beta$  parameters, CT spectra. Spectral properties of Lanthanide and Actinide metal complexes.

#### UNIT-IV

13h

**Magnetic properties of coordination compounds-** Types of magnetism, temperature effect, magnetic susceptibility and its determination- Gouy, Faraday, VSM method. Diamagnetic correction, orbital contribution, spin-orbital coupling, ferro- and antiferromagnetic coupling, spin-crossover. Magnetic properties of Lanthanide and Actinide metal complexes.

**Photochemical reactions of transition metal complexes:** Basic photochemical processes, Kasha's rule, quantum yield, Jablonskii diagrams, photo substitution reactions, photo-redox reactions, ligand photoreactions.

## SUGGESTED BOOKS

1. Advanced Inorganic Chemistry- F. A. Cotton, G. Wilkinson and P. L. Gaus; John Wiley and sons. Inc, 6<sup>th</sup> edition (1999).
2. Chemistry of elements- N. N. Greenwood and A. E. Earnshaw, 2<sup>nd</sup> edition, Butterworth Heinemann (1997).
3. Inorganic Chemistry J. E. Huheey, E. A. Keiter and R. L. Keiter, 4<sup>th</sup> edition; Addison; Wesley (1993).
4. Inorganic Chemistry, D. F. Shriver, P. W. Atkins and C. H. Langford, 5<sup>th</sup> edition, ELBS; Oxford University Press, (2010)
5. Inorganic Electronic spectroscopy, A. B. P. Lever, 2<sup>nd</sup> edition, Elsevier. (1984).
6. Magnetochemistry, R.L. Carlin, Springer Verlag (1986).
7. Electronic Absorption Spectroscopy and related Techniques, D. N. Sathyanarayana, University Press (2001).
8. Inorganic Chemistry A Unified Approach by W. W. Porterfield, Elsevier 2005 2<sup>nd</sup> edition.
9. Inorganic chemistry G L Miessler, P J Fisher and D A Tarr 5<sup>th</sup> edition (2008).

## Ch-202: ORGANIC CHEMISTRY – II

### UNIT-I

#### Aromatic Substitution Reactions

13h

*Electrophilic Substitution Reactions:* The arenium ion mechanism. Orientation and reactivity. Energy profile diagrams. The *ortho/para* ratio, *ipso* attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Effect of leaving group. Amination, sulfonylation reactions; Diazonium coupling, Vilsmeier-Haack reaction, Gatterman reaction, Gatterman-Koch reaction and Hoesch reaction.

*Nucleophilic substitution reactions:* The  $S_NAr$ ,  $S_N1$ , benzyne and  $S_{RN}1$  mechanisms. Reactivity: effect of substrate structure, leaving group and attacking nucleophile. Goldberg reaction, Bucherer reaction, Schiemann reaction, von Richter reaction, Sommelet-Hauser and Smiles rearrangements.

### UNIT-II

#### Addition Reactions

13h

*Addition to carbon-carbon multiple bonds:* mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals. Regio-, stereo- and chemo-selectivities. Orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Addition of alkenes and/or alkynes to alkenes and/or alkynes. Ene synthesis. Michael reaction.

*Addition to carbon-heteroatom multiple bonds:* Mechanism of metal hydride reduction (NaH, LiH,  $LiAlH_4$ ,  $NaBH_4$ ) of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents and organolithium reagents to carbonyl compounds and unsaturated carbonyl compounds. Conversion of aldehydes to nitriles. Hydrolysis of nitriles and addition of amines to isocyanates. Formation of xanthates. Wittig, Mannich and Stobbe reactions.

### UNIT-III

13h

#### **Elimination Reactions**

The E2, E1 and E1cB mechanisms and their spectrum. E2C and E2H mechanisms. Orientation of the double bond. Reactivity-effects of substrate structure, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination reactions (including Chugaev reaction).

#### **Rearrangement Reactions:**

*Carbon-carbon:* Wagner-Meerwein, Pinacol-Pinacolone, Fries, Benzil-benzilic acid and Wolff rearrangement. Arndt-Eistert synthesis and Tiffeneau- Demjanov reaction. Fritsch-Buttenberg-Wiechell, Favorskii, Dienone-phenol and Baker-Venkataraman rearrangement.

*Carbon-nitrogen:* Beckmann, Hofmann, Curtius, Lossen, Schmidt, Stevens, Neber and Benzidine rearrangement.

*Carbon-oxygen:* Wittig rearrangement and Baeyer-Villiger oxidation.

### UNIT-IV

#### **Chemistry of biological molecules - II**

##### **Amino acids and Peptides**

Amino acids essential and non essential. Classification and nomenclature of peptides. Sanger and Edman methods of sequencing. Cleavage of peptide bond by chemical and enzymatic methods. Peptide synthesis- Protection of amino group (Boc-, Z- and Fmoc-) and carboxyl group as alkyl and aryl esters. Use of DCC, EEDQ, HOBt and active esters, in peptide bond formation reactions. Deprotection and racemization in peptide synthesis. solid phase peptide synthesis carbohydrates techniques. Synthesis of oxytocin, and enkephalins.

#### **SUGGESTED BOOKS**

1. Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March, John Wiley (2008).
2. Advanced Organic Chemistry, F A Carey and R J Sundberg Plenum, (2000).
3. A Guide Book to Mechanism in Organic Chemistry, P Sykes, VI edition, Pearson, (2003).
4. Structure and Mechanism of Organic Chemistry, C. K. Ingold, II Edition, CBS, (2016).
5. Organic Chemistry, R T Morrison, R N Boyd and S K Bhattacharjee, VII edition, Pearson, (2018).
6. Principles of Organic Synthesis, III edition), R O C Norman and J M Coxon, Blackie Academic and Professional (Indian Reprint), (2012).
7. Natural Products: their chemistry and biological significance, J Mann, Longman, (2000)
8. Organic Chemistry, Volume I, I L Finar, VI edition, Pearson, (2018).
9. Organic Chemistry, Volume II, I L Finar, VI edition, Pearson, (2018).
10. Organic Chemistry, J Clayden, N Greeves and S Warren, II edition, Oxford University Press, (2014)
11. Name Reactions – A collection of detailed reaction mechanisms, J J Li Springer, (2012)
12. Modern Methods of Organic Synthesis W Carruthers and I Coldham, IV edition, Cambridge University Press, (2015).
13. Peptides Chemistry: A practical text book, M. Bodansky, Springer-Verlag NY, (1988).

14. Solid-phase peptide synthesis: A practical Approach-E. Artherton & R.C. Sheppard, I R L, Oxford Univ. Press, (1989).
15. Peptides: Chemistry and Biology, N Selwad and H.-D. Jakubke, Wiley-VCH, (2002).

## C-203: PHYSICAL CHEMISTRY- II

### UNIT-I

#### **Thermodynamics-I**

13h

Thermodynamics: Concepts of partial molar properties – partial molar free energy, chemical potential, partial molar volume and its significance. Gibbs-Duhem equation, Gibbs-DuhemMargulus equation. Determination of partial molar volume : Graphical method, intercept method and Apparent molar volume method. Concept of fugacity; Determination of fugacity by graphical method and compressibility factor method. Activity and activity coefficient : Determination of activity coefficient by EMF and solubility method. Thermodynamics of nonideal system-Excess thermodynamic function,  $G^E$ ,  $S^E$ ,  $H^E$  etc. Phase Rule : Derivation of phase rule from the concept of chemical potential. Application of Phase Rule to three components system :Principle of triangular diagram : Plots for a mixture of three liquids consisting of one ,two and three pairs of partially miscible liquids. Statistical Thermodynamics: Objectives of statistical thermodynamics, Concept of distributions, Types of ensembles. Thermodynamic probability, Most probable distribution Law – Partition Function, (Definition and significance): Molar and molecular partitions- translational, rotational, vibrational and electronic partition functions- Relation between thermodynamic functions (  $E$ ,  $H$ ,  $S$ ,  $G$  and  $C_v$  ) and the partition functions.

### UNIT-II

#### **Thermodynamics-II**

13h

Sackur-Tetrode equation for entropy of translation function. Relation between equilibrium constant and partition function. Different Distribution Laws:Types of Statistics : Maxwell – Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Derivation of the equations for above three distribution Laws. Comparison of Bose-Einstein and Fermi-Dirac statistics with Maxwell – Boltzmann statistics. Problems and their Solutions.

Non-equilibrium Thermodynamics : Thermodynamic criteria for non-equilibrium states- Phenomenological Laws and Onsager's reciprocity relations, Coupled and Non-coupled reactions, Entropy production and entropy flow. Electro kinetic Phenomenon. Postulates and methodologies: Uncompensated heat and thermodynamics fuction production. deDonder's inequality. Rate of entropy production. Transformations of the generalized fluxes and forces :eg., Chemical reaction, heat flow, Diffusion or material flow, flow of electric current.

### UNIT-III

#### **Electrochemistry-I**

13h

Elctrochemistry of solutions: Ionic atmosphere, Debye-Huckel theory for the problem of activity coefficient, Debye-Huckel limiting Law, Debye-Huckel equation for appreciable concentration, Debye-HuckelOnsagar conductance equation and its extension to ion solvent

interactions, Debye-HuckelBjerrum mode, Ion association, triple ions, triple ions and conductance minima. Thermodynamics of electrified interface, derivation of electro capillary Lipmann's equation, surface excess, thermodynamic aspects of surface excess. The method of determination and measurement of interfacial tension as a function of applied potential difference across the interface.

## UNIT-IV

### **Electrochemistry-II**

#### **13h**

Structure of electrified interface: Helmholtz theory, Guoy- Chapman theory, Stern model. Overpotential: Concentration, activation and ohmicoverpotential; Derivation of Butler- Volmer equation.

Semiconductor- solution interface: Theory of double layers at semiconductor- electrolyte interface.

Electrocatalysis: Definition and Influence of various parameters. Quantum aspects of charge transfer at electrode solution interface, quantization of charge transfer, tunneling of electrons for hydrogen evolution with reference to electrocatalysis.

Polarography technique-Principle, DME- Merits and limitations, experimental, polarogram, half wave potential, diffusion controlled current, Ilkovic equation (no derivation), qualitative and quantitative estimation of metal ions.

Advanced Electrodes: Rotating disc electrodes, Membrane electrodes (Definition, examples with diagrams and applications to each), carbon electrodes.

## **SUGGESTED BOOKS**

1. Molecular thermodynamics, Donald A. Mc Quarrie, John D. Simon University Science Books California, (1999).
2. Thermodynamics for Chemists by S. Glasstone, East-West Press, New Delhi, (1960).
3. Thermodynamics, by Rajaraman and Kuriacose, East-West Press, (1986).
4. Statistical Thermodynamics, M. C. Gupta (Wiley Eastern Ltd.) 1993.
5. Elements of Classical and Statistical Thermodynamics, L. K. Nash, Addison-Wiley (1979).
6. Thermodynamics, Statistical Thermodynamics and Kinetics by Thomas Engel & Philip Reid, Pearson Education inc. (2007).
7. Modern Electrochemistry Vol-1 and 2, J. O. M. Bockris and A. K. N. Raddy, Plenum, New York (1978).
8. An introduction to electrochemistry: Samuel Glasstone East-West, edition New Delhi (1942)
9. Text book of physical chemistry Samuel Glasstone, 2nd edition, Mac Millan India Ltd (1991)
10. Principles and applications of Electrochemistry- D. R. Crow 3rd edition, Chapmanhall London (1988).
11. Physical chemistry through problems by S K Dogra and S Dogra, Wiley Eastern Ltd., 4<sup>th</sup> Edn. 1993.
12. Electrochemical methods by A J Bard and I R Faulkner, 2<sup>nd</sup> Edn., Wiley New York, 2000.

## Ch-204: MOLECULAR SPECTROSCOPY

### UNIT-I

#### **Symmetry and Group Theory in Chemistry**

Definition of groups, subgroups, cyclic groups, conjugate relationships, classes, simple theorems in group theory. Symmetry elements and symmetry operations, point groups, Schönflies notations, representations of groups by matrices, reducible and irreducible representations, characters of representations, Great Orthogonality Theorem (without proof) and its applications, character tables and their uses (representations for the  $C_n$ ,  $C_{nv}$ ,  $C_{nh}$ ,  $D_{nh}$  etc groups to be worked out explicitly) Mulliken symbols for irreducible representations. Direct products, Applications of group theory to quantum mechanics identifying non-zero matrix elements, derivation of the orthonormalization conditions.

### UNIT-II

#### **Unifying principles**

Interaction of electromagnetic radiation with matter- time-dependent perturbation theory, transition moment integral, selection rules- symmetry and spin forbidden transitions.

#### **Infrared Spectroscopy-I**

Vibrations of molecules, harmonic and anharmonic oscillators- vibrational energy expression, energy level diagram, vibrational wave functions and their symmetry, selection rules, expression for the energies of spectral lines, computation of intensities, hot bands, effect of isotopic substitution

Diatomic vibrating rotor, Born-Oppenheimer approximation, vibrational-rotational spectra of diatomic molecules, P, Q and R branches, breakdown of the Born-Oppenheimer approximation.

#### **Infrared Spectroscopy-II**

Vibrations of polyatomic molecules: Normal coordinates, translations, vibrations and rotations, vibrational energy levels and wave functions, fundamentals, overtones and combinations. Vibration-rotation spectra of polyatomic molecules- parallel and perpendicular vibrations of linear and symmetric top molecules. Techniques and instrumentation, FTIR

### UNIT-III

#### **Microwave Spectroscopy**

Rotations of molecules, rigid diatomic molecule- rotational energy expression, energy level diagram, rotational wave functions and their symmetry, selection rules, expression for the energies of spectral lines, computation of intensities, effect of isotopic substitution, centrifugal distortion and the spectrum of a non-rigid rotor.

Rotational spectra of polyatomic molecules- linear, symmetric top and asymmetric top molecules, Stark effect, techniques and instrumentation.

#### **Raman Spectroscopy**

Classical theory of the Raman effect, polarizability as a tensor, polarizability ellipsoids, quantum theory of the Raman effect, Pure rotational Raman spectra of linear and asymmetric top

molecules, vibrational Raman spectra, Raman activity of vibrations, rule of mutual exclusion, rotational fine structure- O and S branches, Polarization of Raman scattered photons Structure determination from Raman and IR spectroscopy-AB<sub>2</sub> and AB<sub>3</sub> molecules Techniques and instrumentation

#### **UNIT-IV**

##### **Electronic Spectroscopy**

Born-Oppenheimer approximation, vibrational coarse structure, intensities by Franck-Condon principle, Dissociation energy, rotational fine structure, Fortrat diagram, pre-dissociation

Electronic structure of diatomic molecules- basic results of MO theory, classification of states by electronic angular momentum- $\sigma$ ,  $\pi$ ,  $\delta$ , and  $\phi$  molecular orbitals, selection rules, spectrum of singlet and triplet molecular hydrogen

Electronic spectra of polyatomic molecules- localized MOs, spectrum of HCHO, change of shape on excitation

Decay of excited states- radiative (fluorescence and phosphorescence) and non-radiative decay, internal conversion

#### **SUGGESTED BOOKS**

1. Chemical Applications of Group Theory, F. A. Cotton, Wiley Eastern (1976).
2. Molecular Symmetry, D. S. Schonland, Van Nostrand (1965).
3. Introduction to Molecular Spectroscopy, C. N. Banwell, TMH Edition (1994).
4. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw Hill (Int. Students Edition) (1988).
5. Molecular Spectroscopy, J. D. Graybeal, McGraw Hill (Int. Students Edition) (1990).
6. Spectroscopy, Vols. 1-3, B. P. Straughan and W. Walker, Chapman Hall (1976).

## Ch-205: GREEN SYNTHESIS (SOFT CORE)

36 h

### UNIT-I

#### **Use of ultrasound and Microwaves in organic Synthesis**

12 h

*Use of ultrasound:* Introduction, instrumentation, the phenomenon of cavitation. Sonochemical esterification, substitution, addition, alkylation, oxidation, reduction and coupling reactions.

*Use of microwaves:* Introduction, concept, reaction vessel/medium, specific effects, atom efficiency (% atom utilization), advantages and limitations. N-alkylation and alkylation of active methylene compounds, condensation of active methylene compounds with aldehydes and amines. Diels-Alder reaction. Deprotection of esters and silyl ethers. Oxidation of alcohols and sulfides.

*Ionic-liquids:* Introduction, structure, synthesis and applications of some important ionic liquids in organic synthesis.

### UNIT-II

#### **Polymer supported reagents in organic synthesis**

12 h

Introduction- properties of polymer support, advantages of polymer supported reagents and choice of polymers. Applications.

*Substrate covalently bound to the support:* Synthesis of oligosaccharides, Dieckmann cyclisation. Preparation of polymer bound aldehyde and application in aldol and Wittig reactions. Synthesis of polystyrylboronic acid and use in diol protection reaction.

*Reagent linked to a polymeric material:* Preparation of sulfonazide polymer and application in diazotransfer reaction. Synthesis of polymer bound per acid and its applications.

Polymer supported catalytic reactions: Preparation of polymer supported  $AlCl_3$  and application in etherification and acetal formation reactions.

#### **Phase transfer catalysis and Crown ethers**

Phase transfer catalysis: Introduction, definition, mechanism of phase transfer catalysis. Types of phase transfer catalysts and reactions and their Advantages.

Preparation of catalysts and their application in substitution, elimination, addition, alkylation, oxidation and reduction reactions.

Crown ethers: Introduction, nomenclature, features, nature of donor site. General synthesis of Crown ethers.

Synthetic applications: Alkylation, generation of carbenes, aromatic substitution and displacement reactions. Generation and application of superoxide anions. Cation deactivation reactions.

### UNIT-III

#### **Multi-component Reactions**

12 h

Studies on the mechanistic aspects and use of the following reactions in organic synthesis: Passerini-Ugi; Hantsch; Biginelli; Doebner-Miller; Ritter; Jacobson; Betti; Robinson-Schopf; Barbier; Baylis-Hilman; Petasis; Ivanov and Suzuki coupling reaction.

## SUGGESTED BOOKS

1. Some modern methods of Organic Synthesis, W. Caruthers, Cambridge Univ. Press London, 2<sup>nd</sup> Edition, 1998.
2. Organic synthesis: Special techniques, V. K. Ahluwalia and R. Aggarwal, Narosa, New Delhi, 2003.
3. Green Chemistry, environment friendly alternatives, R. Sanghi and M. M. Srivastava, Narosa, New Delhi, 2003
4. Green Chemistry-an introductory text, M. Lancaster, Royal Society of Chemistry, UK, 2003.
5. Organic chemistry Vol. 2, 6<sup>th</sup> Edition, I. L. Finar, Longman, 1992.
6. Crown ethers & cryptands, G. W. Gokel, Royal Society of Chemistry, UK, 1991.
7. Macrocyclic Polyether Chemistry, G. W. Gokel, S. M. Korzeniowski, Vol 1 to3, Wiley, NY, 1978, 1981, 1987.
8. Phase Transfer Catalysis in Organic Synthesis, W. B. Weber, G. W. Gokel, Springer, Berlin, 1977.
9. Phase Transfer Catalysis, E. V. Dehmlov, S. S. Dehmlov, 2<sup>nd</sup> Edn., Verlag chemie, Wienheim, 1983.
10. Polymers as aids in Organic synthesis, N. K. Mathur, C. K. Narang and R.E. Williams, Academic Press, NY, 1980.

## Ch -205: PHOTO CHEMISTRY (SOFT CORE)

### UNIT-I

12h

Importance of Photochemistry, Laws of Photochemistry: Grothus –Draper Law, Stark-Einsteins Law, Laws of light absorption, Quantum yield and numerical problems. Photochemistry and spectroscopy, units and dimensions. Electronic energy states of atoms, term symbols for atoms, energy levels for the electronic configuration of carbon and oxygen illustrating spin orbit coupling and Hunds rules, inverted multiplets as applied to simple atoms and also for inner transition metals, Laporte's selection rules. Physicochemical Properties of electronically excited molecules: Nature of changes on electronic excitation: acidity, dipole moment, redox potentials etc. Fates of excited species, Electronic, vibrational, rotational energies-potential energies diagram. Shapes of absorption band and Franck Condon principle.

### UNIT-II

12h

Quantum mechanical formulation of Franck Condon, crossing of potential energy surfaces, Non crossing rule of Teller for potential energy surface. Emission spectra, fluorescence and phosphorescence Environmental effect on absorption and emission spectra, solvent red shift and blue shift in absorption spectra. Experimental techniques to determine the intermediates in photochemical reactions Classification of photochemical reactions, Rate constants and life times of reactive energy state Effect of light intensity on the rate of photochemical reaction.

### UNIT-III

12h

Photosensitized reactions: photodissociation-Gas phase photolysis, photofragmentation in liquid phase, photodegradation of polymers, Isomerization and other rearrangement reactions, Atmospheric photochemistry.

Photoelectrochemistry: Introduction, efficiency of conversion of light to chemical and electrical

energy, frequently measured quantities. Photosplitting of water using colloidal suspensions.  
Semi conductors: Bonding, conductivity, mechanism of conductivity, energy bands in semiconductors; impurity semiconductors.  
Photo voltaic effect: p-n junction, solar cells, silicon cells, GaAs solar cells, schottky barrier solar cells.  
Photocatalysis: Photocleavage of environmentally hazardouswaste matter by using TiO<sub>2</sub>, ZnO and MgO. Photooxidation and photoreduction reactions.

### **SUGGESTED BOOKS**

1. Fundamentals of photochemistry, K.K. RohatgiMukherjee, Wiley Eastern Limited (1986)
2. Photochemistry, Carol E Wayne and Richard P Wayne, Oxford University Press (1996)
3. Introduction to Semiconductor Materials and devices M S Tyagi, John Wiley and sons (1991)
4. Organic Photochemistry, J. M. Cozen and B. Halton, Cambridge University Press (I st Edition) 1974.
5. Molecular Reactions and Photochemistry, C H Deputy and D S Chapman, Prentice Hall India, New Delhi ( 1st Edition) , 1972.
6. Concepts of Inorganic photochemistry, A. W. Adamson and P D Fleischaves, John Wiley & Sons Inc. (1975).
7. Physical Chemistry, P. W. Atkins, Julio de Paulo ELBS 7th Edition (2002)

### **Ch- 206, 207, 208, 209 Practicals**

**(4 hrs per day, 4 days per week)**

**Inorganic Chemistry Practicals - I, II, III & IV  
Organic Chemistry Practicals - I, II, III & IV  
Physical Chemistry Practicals - I, II, III & IV**

Experiments are as in first semester. Every student will carry out experiments in each of the three branches of chemistry on a rotation basis from 1<sup>st</sup> to 3<sup>rd</sup> Semester.

**THIRD SEMESTER**  
**INORGANIC CHEMISTRY SPECIALISATION**

**Ch-301 IC: INORGANIC REACTION MECHANISMS AND BIOINORGANIC CHEMISTRY**

**52 Hours**

**UNIT-I**

**13h**

**Reaction mechanism-** Labile, inert, stable and unstable complexes, classification of mechanisms- energy profile of reactions having different mechanisms.

**Substitution in square planar complexes-** mechanism, factors affecting substitution, trans-effect, theories of trans-effect, application of trans-effect in the synthesis of complexes.

**Mechanism of ligand substitution in octahedral complexes-** kinetics, factors affecting substitution in octahedral complexes: Leaving group, chelate and metal effects.

**Acid-Base catalysis:** Acid catalysed aquation and anation reactions, conjugate base hydrolysis-SN<sub>1</sub>CB mechanism, stereochemistry of octahedral substitution.

Application of ligand substitution reactions for the synthesis of octahedral complexes.

**UNIT-II**

**13h**

**Electron transfer reactions-** complementary and non-complementary, outer sphere electron transfer- Marcus equation, Inner sphere electron transfer- one and two electron transfer, use of electron transfer reactions for the synthesis of complexes.

**Oxidative addition- reductive elimination, migratory insertion reactions.**

**Metal ions in biological system-** Metal ligand interactions with DNA. Metal ion deficiency and treatment (Fe, Zn, Cu, Mn); toxicity of Fe, Cu, Heavy metals- As, Hg, Pb and Cd; detoxification; chelation therapy; metal complexes as anticancer and antiarthritic drugs. Biological roles of Ca: Binding sites of Ca<sup>2+</sup> in proteins, importance of Ca<sup>2+</sup> in muscle contraction and in blood clotting process.

**UNIT-III**

**13h**

**Metal ion transport across cell membranes;** Na<sup>+</sup>/K<sup>+</sup> transport, Na<sup>+</sup>/K<sup>+</sup> pump, ionophores, crown ethers.

**Iron storage and transfer-** ferritin, transferrin and siderophores.

**Oxygen transport and oxygen uptake proteins-** transport and storage of dioxygen; Heme proteins and oxygen uptake, structure and functions of haemoglobin and myoglobin, dioxygen binding, Bohr effect, Hill equation, role of distal and proximal histidine; Model complexes for dioxygen binding, non- porphyrin systems- hemerythrin and hemocyanin.

**Nitrogen fixation:** Nitrogenase: structural aspects and functions, abiological nitrogen fixation.

**Photosynthesis:** Chlorophyll- structural features, role of Mg<sup>2+</sup>- Z scheme of photosynthesis- PSI and PSII.

**UNIT-IV**

**13 h**

**Structure and functions of metalloproteins in electron transfer process -** Cytochromes, ferridoxines- 2Fe-2S, Rieske centers, high potential iron proteins; 4Fe-4S, 3Fe-4S, 8Fe-8S and

rubredoxin. Mitochondrial flow of electrons from NADH to oxygen, cytochrome C, Cytochrome C oxidase.

**Metalloenzymes: Structure and reactivity -**

Zinc enzymes: carboxypeptidase, carbonic anhydrase and alcohol dehydrogenase.

Cu enzyme: superoxide dismutase.

Mo enzyme: Xanthine oxidase and nitrate reductase.

Fe enzymes: catalase, peroxidase and cytochrome P-450.

**Vitamin B<sub>12</sub> Coenzyme:** B<sub>12r</sub>, B<sub>12s</sub>, biochemical functions of cobalamins; Biomethylation, mutase activity.

**SUGGESTED BOOKS**

1. Inorganic and organometallic reaction mechanism; J. D. Atwood; Brooks/cole publication co. 1985.
2. Reaction mechanism of inorganic and organometallic systems; J. B. Jordon, Oxford University Press 2<sup>nd</sup> edition, 1998.
3. Inorganic Chemistry, 3<sup>rd</sup> Edition; Gary. L. Miessler and Donald . A. Tarr, Pearson education Inc 2007.
4. Inorganic Chemistry; K. F. Purcell and J. C. Kotz, Saunders company, 1977.
5. Bio-inorganic chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, Viva Books Pvt. Ltd 1998
6. Bioinorganic Chemistry; Asim. K. Das; Books and allied (p) Ltd., 2007.
7. Advance Inorganic reaction mechanism G. Whitmore IVY Publishing house Delhi 2010.
8. Bioinorganic chemistry: Inorganic elements in the chemistry of life Wolfgang Kaim and Brigitte Schwederski Wiley India edition 2012.
9. Principles of Bioinorganic Chemistry; S. J. Lippard and J. M. Berg; Panima Pub. Corporation 1997.

**Ch – 302 IC: ADVANCED ANALYTICAL TECHNIQUES**

**52 Hours**

**UNIT-I**

**13h**

**Absorption Spectroscopy:** absorption, emission, fluorescence phenomenon, principles and differences, Flame AAS, Instrumentation, different types of nebulizers, Nonflame techniques, GAAS, electrothermal vapourisers, graphite furnace, cold vapour AAS, radiation sources, HCL, EDL, TGL etc. detectors, photoemmissive cells, PMT, photodiodes, Interferences, spectral, chemical, matrix, background absorption, correction methods, deuterium arc, zeeman effect, Smith-Hieftje methos, single beam and double beam instruments, evaluation procedures, applications of AAS.

**UNIT-II**

**13h**

**Atomic Emission Spectroscopy:**Emission-principle, Inductively coupled plasma optical emission spectrometry, theory, ICP characteristics, sample introduction methods, torch configuration and view modes, analytical performance.merits and limitations of AES over AAS, Detection limit, application to elemental analysis, Mass spectrometry in the analysis of inorganic compounds different techniques, applications

**Electroanalytical Techniques-I** Electrode Potential, Currents in Electrochemical cells, Potentiometric titrations. Electrogravimetry-faraday's laws of electrolysis, Coulometry, Coulometric titrations.

### UNIT-III

13h

#### **Electroanalytical Techniques-II:**

Voltammetry- principle, DME-advantages,limitations, Hydrodynamic Voltammetry, Cyclic voltammetry-principle, conditions for reversible, quasi reversible and irreversible reactions Anodic stripping voltammetry-principle and applications, Polarography, Pulse polarography, Amperometry-titrations, different titration curves,applications, numerical problems on all these techniques.

**Thermal Methods of Analysis:** Principle, methodology and applications: thermogravimetric and differential thermal analysis, differential scanning calorimetry; Thermo-mechanical and dynamic mechanical analysis ; thermometric titrations. Thermal stability of polymers, applications, decomposition patterns, decomposition reactions-examples.

### UNIT-IV

13h

**Analysis of Biomolecules:** Introduction, single biomolecule detection and characterization, Fluorescence, principle, factors influencing fluorescence, fluorescence based biosensors, Fluoroimmunosensors.

Mass spectrometry-principle, sample preparation, probe tip, MALDIMASS, types of ion separation, instrumentation-types, applications in structural biology, Application of NMR spectroscopy in the analysis of biomolecules. Raman spectroscopy- phenomenon, merits and limitations, application to biomolecules, Voltammetry in Vivo for chemical analysis of neurotransmitters in central nervous system

#### **SUGGESTED BOOKS**

1. Analytical Chemistry. Gary D Christian, 5th Edition, John – Wiley and Sons Inc., (1994)
2. Fundamentals of Analytical Chemistry.D. A. Skoog, D. M. West and F. J. Holler, 7th Edition, Saunders College Publishing (1996).
3. Instrumental methods of Analysis.H. H. Willard, L. L. Merrit , J. A. Dean and F. A. Set, CBS Publishers (1996).
4. Instrumental methods of Chemical Analysis, G. W. Ewing, 5th edition, McGraw-Hill, New York, 1988.
5. Electrochemical methods: A.J. Bard & I. R. Faulkner, 2<sup>nd</sup> edition, Wiley, New York, 2000.
6. Vogel's text book of Quantitative Chemical analysis 5<sup>th</sup> edition, Ed., Jeffery et. al ELBS/Longman, 1989
7. Encyclopedia of Analytical Chemistry: Ed. By R.A. Meyers Vol. 1 – 15, John Wiley, 2000.
8. Fundamentals of Instrumental Analysis, Skoog, D. M. West and F. J. Holler, 8th Edition, Saunders College Publishing (2004).

### **Ch-303 IC/OC/PC: ORGANIC SPECTROSCOPY (Common to Inorganic/ Organic/ Physical chemistry)**

52 Hours

#### UNIT-I

13h

#### **Ultraviolet/ visible spectroscopy**

Instrumentation. Classification of electronic transitions. Substituent and solvent effects.

UV spectral study of alkenes, polyenes,  $\alpha,\beta$ -unsaturated carbonyl and aromatic compounds. Empirical rules for calculating  $\lambda_{\max}$ .

### **Vibrational Spectroscopy: Infrared and Raman spectroscopy**

Instrumentation. Sampling techniques, Group frequencies, factors affecting group frequencies, Bond order, Mass effect, Conjugation, Inductive, resonance, steric effects. Intramolecular interactions. Application of IR in the study of H-bonding, stereoisomerism and tautomerism. Complementarity of IR and Raman. Identification of the following organic compounds by IR: alkanes, alkenes, alkynes, aromatic compounds, aldehydes, ketones, alcohols, acids, acid chlorides, amides, amines, esters, halides and nitro compounds etc. Problems using UV and IR.

## **UNIT-II**

13h

### **Nuclear magnetic resonance spectroscopy-I**

Introduction, Magnetic properties of nuclei- Resonance condition. Nuclear spin, population of nuclear spin levels and NMR isotopes, Relaxation methods. Instrumentation and sample handling, FT-NMR.

Chemical shift. Mechanism of shielding and deshielding in Alkanes, Alkyl halides, Alkenes, Aromatic compounds, Carbonyl compounds and Annulenes. Pascal's triangle-low and high resolution, spectrum of ethanol. Karplus Curve, Diamagnetic and paramagnetic effects and magnetic anisotropy. Equivalence of protons-chemical and magnetic equivalence. Spin-systems: First order and second order coupling of AB systems, Simplifications of complex spectra.

Problems.

Spin-spin interactions: AX, AX<sub>2</sub>, AX<sub>3</sub>, AMX, AB types. Vicinal, geminal and long range coupling-Spin decoupling. Chemical shift reagents and deuterium exchange. Stereochemistry and hindered rotations. Temperature effects.

## **UNIT-III**

13h

### **Nuclear magnetic resonance spectroscopy-II**

CIDNP, Nuclear Overhauser effect (NOE). Factors influencing coupling constants and Relative intensities. Protons attached to elements other than carbon.

<sup>13</sup>C NMR Spectroscopy: Range and factors affecting chemical shifts of alkanes, alkyl halides, alkenes, alcohols, ethers, alkynes, carbonyl compounds and aromatics..

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

Explanation of the principle, applications to structure elucidation and stereochemistry of simple organic molecules.

Dynamic NMR.

NMR spectroscopy of other nuclei with spin  $I = \frac{1}{2}$ . Introduction to <sup>15</sup>N, <sup>19</sup>F, <sup>29</sup>Si and <sup>31</sup>P NMR spectroscopies.

## **UNIT-IV**

13h

### **Mass spectrometry and Composite Problems:**

Basic principles-instrumentation – ion production-ion analysis-magnetic sector instruments Quadrupole mass spectrometers. Time of flight mass spectrometers-ion cyclotron resonance spectrometers- Mass spectrum-molecular ion-types of ions in mass spectra and effects of

isotopes on mass spectra. Methods of ionization, EI, FAB MALDI and ESI methods. Fragmentation of alkanes, alkenes, aromatics, alkyl halides, alcohols, aldehydes, ketones, acids, esters, ethers, amines, nitro and halo compounds peptides, Nitrogen rule, Factors affecting cleavage patterns. McLafferty rearrangement. Determination of molecular formula. Problems. Use of HRMS to determine exact molecular formulae of compounds. Application of UV, IR, NMR and MS methods and chemical reactions in the structure elucidation of organic compounds – composite problems.

### SUGGESTED BOOKS

1. Spectroscopic methods in organic chemistry, 7<sup>th</sup> edition, D Williams and I Fleming, Springer International Publishing, Berlin – 2019
2. Fundamentals of molecular spectroscopy 5<sup>th</sup> edition, C N Banwell, E M McCash, H K Choudhury, Tata McGraw Hill, New Delhi - 2015
3. Spectrometric identification of organic compounds, R. M. Silverstein, F X Webster, D J Kiemle and D L Bryce, 8<sup>th</sup> Wiley student edition, New Delhi, 2015.
4. Organic spectroscopy, W. Kemp, Macmillan, London, 2011.
5. Introduction to spectroscopy, 4<sup>th</sup> edition, D. L. Pavia, G. M. Laupman and G. S. Kriz, Harcourt College Publishers, 2009.
6. Structure determination of organic compounds E Pretsch, P Buhlmann and M Badertscher, Springer-Verlag, Berlin – 2009.
7. Spectroscopic methods in organic chemistry, M Hesse, H Meier, B Zeeh, 2<sup>nd</sup> edition, Thieme, Stuttgart, 2008.
8. Organic Spectroscopy, LDS Yadav, Springer/Kluwer, 2005.
9. Organic Spectroscopic Analysis, R J Anderson, D J Bendell, P W Groundwater, RSC, Cambridge, 2004.
10. Mass spectrometry a foundation course, K Downard, RSC, Cambridge, 2004.
11. Structural analysis of organic compounds by combined application of spectroscopic studies, J T Clerc, E Pretsch, J Seibl, Elsevier, Amsterdam, 2001.
12. Biomolecular NMR Spectroscopy, J N S Evans, Oxford University, Oxford, 1995.
13. Modern NMR techniques and their Applications, Ed. A I Popov, Marcel Dekker, 1991.
14. Instrumental methods of analysis, H. H. Willard, L. L. Merritt, J. A. Dean and F.A. Settle, 7<sup>th</sup> edition, CBS Publishers and Distributors, 1989
15. Organic mass spectroscopy, K. R. Dass & E. P. James, IBH New Delhi, 1976.
16. The IR Spectra of complex molecules, Vols. I and II, L J Bellamy, Chapman and Hall, London, 1975.
17. Mass spectrometry of organic compounds, H. Budzkievicz, Djerassi C. and D. H. Williams, Holden-Day New York, 1975.
18. Interpretation of organic mass spectra, F W McLafferty, W A Benjamin, London, 1973.
19. Organic spectroscopy, P. Laszlo and P. Stang, Harper & Row, New York, 1971.
20. Applications of absorption spectroscopy to organic compounds, J. R. Dyer, Prentice-Hall, New Delhi, 1969.
21. Interpretation of the UV spectra of natural products, A.I. Scott, Pergamon Press, Oxford, 1964.

**C-304-[OPEN ELECTIVE, NON-CHEMISTRY PAPER]**

**OPEN ELECTIVE FOR NON-CHEMISTRY STUDENTS**  
**Ch-304 OE: CHEMISTRY IN DAILY LIFE**

**52 Hours**

**UNIT-I**

**13h**

**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, disulphites,

**Artificial sweeteners:** aspartame, saccharin, dulcin, sucralose and sodium cyclamate.

**Flavours:** Vanillin, alkyl esters (fruit flavours) and monosodium glutamate.

**Artificial food colorants:** Coal tar dyes and non-permitted colours and metallic salts. Analysis of pesticide residues in food.

**Paints & Pigments:** White pigments (white lead, ZnO, lithopone, TiO<sub>2</sub>). Blue, red, yellow and green pigments. Paints and distempers: Requirement of a good paint. Emulsion, latex; luminescent paints. Fire retardant paints and enamels, lacquers. solvents and thinners for paints.

**Dyes:** Colour and constitution (electronic concept). Classification of dyes. Methods of applying dyes to the fabrics. A general study of azo dyes, Mordant brown, Congo red and methyl orange.

**UNIT II**

**13h**

**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.

**Composition of soil** – inorganic and organic components in soil-micro and macronutrients.

**Fertilisers:** Classification of Fertilizers- Straight Fertilizers, Compound/Complex Fertilizers, Fertilizer Mixtures. Manufacture and general properties of Fertilizer products- Urea and DAP.

**UNIT-III**

**13h**

**Carbohydrates:** Structure, function and Chemistry of some important mono and disaccharides.

**Vitamins:** Classification and Nomenclature. Sources, deficiency diseases and structures of Vitamin A, Vitamin B, Vitamin C, Vitamin D, Vitamin E & Vitamin K.

**Drugs:** Classification and nomenclature.

Structure and function of: *Analgesics* – aspirin, paracetamol;

*Anthelmintic drug:* mebendazole;

*Antiallergic drug:* Chlorpheniramine maleate,

*Antibiotics:* Penicillin V, Chloramphenicol, Streptomycin.

*Anti-inflammatory agent:* Oxyphenbutazone,

*Antimalarials:* Primaquine phosphate & Chloroquine.

**Oils and fats:** Composition of edible oils, detection of purity, rancidity of fats and oil. Tests for adulterants like argemone oil and mineral oils.

**Soaps & Detergents:** Structures and methods of use of soaps and detergents.

**Chemical Thermodynamics:** Concept of fugacity and free energy, Activity and activity coefficient, spontaneity of processes- entropy and free energy changes. Partial molar quantities, colligative properties, Le-Chatelier principle, phase equilibria. Enzyme catalysed reactions.

**Principles of Reactivity:** Basis kinetic concepts, rates of simple and complex chemical reactions, empirical rate equations. Temperature dependence of rates and activation parameters. Branched chain reactions – explosion limits. Oscillatory reactions.

**Corrosion:** Types and prevention, corrosion failure and analysis

**Chemical energy system** and limitations, principles and applications of primary & secondary batteries and fuel cell. Basics of solar energy, future energy storer.

**Polymers :** Types and classification of polymers. Source and general characteristics of natural and synthetic polymers. Typical examples of polymers used as plastics, in textiles, in electronic and automobile components, in the medical and aerospace materials. Problems of plastic waste management. Strategies for the development of environment friendly polymers.

### **SUGGESTED BOOKS**

1. B. K. Sharma: introduction to Industrial Chemistry, Goel Publishing, Meerut (1998)
2. Medicinal Chemistry by Ashtoush Kar.
3. Drugs and Pharmaceutical Sciences Series, Marcel Dekker, Vol. II, INC, New York.
4. Analysis of Foods – H.E. Cox: 13. Chemical Analysis of Foods – H.E.Cox and Pearson.
5. Foods: Facts and Principles. N. Shakuntala Many and S. Swamy, 4<sup>th</sup> ed. New Age International (1998)
6. Physical Chemistry – P I Atkins and J. de Paula – 7<sup>th</sup> Ed. 2002, Oxford University Press.
7. Handbook on Fertilizer Technology by Swaminathan and Goswamy, 6<sup>th</sup> ed. 2001, FAI.
8. Organic Chemistry by I. L. Finar, Vol. 1 & 2.
9. Polymer Science and Technology, J. R. Fried (Prentice Hall).

**Ch- 401 IC/PC: SOLID STATE CHEMISTRY**  
(Common to Inorganic and Physical chemistry)

**52 Hours**

**UNIT-I**

**Electronic structure of solids**

**13h**

Free electron theory of solids, results of free electron theory; limitations and success of free electron theory, Fermi distribution, Fermi sphere, volume of Fermi sphere, expression for energy levels in a solid, density of states, expression for the number of energy levels in a Fermi sphere.

**Electrical and Magnetic properties of Solids**

Electronic conductivity: Ohm's law, derivation of Ohm's law, Hall Effect, Band theory, Zone theory, Brillion zones, K-space, k-vector, Significance of k-vector, Semiconductors: Energy bands in a semi conductor, temperature dependence of conductivity in metals and semi conductors, intrinsic and extrinsic semiconductors, Insulators; properties, Piezo and inverse Piezo electric effect. Pyroelectricity, Magnetic properties

**UNIT-II**

**13h**

**Heat Capacity of Solids**

Definition, Theories of heat capacity of solids: Dulong-petit, Einstein's theory, Debye Theory. Problems and their solution

**Defects in Solids**

Point defects, Schottky, Frenkel and interstitial, Line defects and Plane defects, Stacking faults and grain boundaries

**Superconductivity**

Superconductivity, BCS theory, Meisner effect, Type I and type II superconductors, Features of superconductors, Frolich diagram, Cooper pairs, Theory of low temperature superconductivity, *Junctions using superconductors*

**Phase Transition in Solids**

Definitions, Classification of phase transitions, First and second order phase transitions: *Martensitic transition, order-disorder transitions and spinodal decomposition*

**UNIT-III**

**13h**

**Geometric Crystallography**

Symmetry elements, Bravais lattices, Screw axes and glide planes, point groups, and space groups and nomenclature. Law of Interfacial angle (Euler's construction).

**Diffraction theory and Single crystal X-ray diffraction**

X-rays, Bragg's law, assignment of lines, diffraction pattern of a primitive cubic lattice, space group extinctions, Scattering factor and structure factor, intensities from atomic positions for BCC and FCC lattices; Ewald's sphere of reflection, Reciprocal Lattice concept, Electron density function, Fourier synthesis, Fourier transform of the structure factor, Phase problem and Patterson synthesis.

**UNIT-IV**

**13h**

**Experimental Methods**

Rotation, Oscillation, Weissenberg and Precession methods. Debye-Scherrer method (Powder method), Determination of lattice parameters from these methods.

**Electron diffraction:**

Experimental technique, Wierl equation, Radial-Distribution method.

**Neutron diffraction**

Principle and Theory, advantages and uses.

**SUGGESTED BOOKS**

1. Introduction to Solids, L. V. Azaroff, McGraw Hill Book Co., New York, 1960.
2. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Holt Saunders International Ltd. New York 1976.
3. Physical Chemistry, G. M. Barrow, McGraw Hill (2nd ISE) 1966.
4. An Introduction to X-ray Crystallography, M. M. Woolfson, Cambridge University Press-Vikas Publishing House, New Delhi 1980.
5. Principles of the Solid State, H. V. Kheer, Wiley Eastern Ltd., New Delhi 1993.
6. Vibrational Spectroscopy of Solids, P.M.A. Sherwood, Cambridge University Press, Cambridge, 1972.
7. Phase Transitions, C.N.R. Rao and K.J. Rao, McGraw Hill Book Co, Newyork 1978.
8. X-ray Structure determination: A practical guide, George H Stout and Lyle H Jenson, John Wiley & sons Newyork 1989.
9. Crystal structure analysis for chemists and biologists J.P Glusker, M.Lewis and M.Ross. Wiley-VCH 1994.

**Ch 402 IC: ORGANOMETALLIC CHEMISTRY AND CATALYSIS**

**52 Hours**

**UNIT-I**

**13h**

**Organometallic complexes-** Stability and decomposition pathways, classification of ligands, nomenclature of organometallic complexes, 16 and 18 electron rules. Electron counting covalent and ionic models. Counting of electrons and finding metal-metal bonds.

**Organotransition metal complexes:** Synthesis structure, bonding and reactivity of multiple metal carbon bonded compounds-Carbenes and carbynes. Synthesis structure and bonding in alkenes, alkynes, allyl moieties, butadiene, cyclobutadiene, cyclopentadiene, arenes, cycloheptadienyl and cyclooctatetraene moieties.

Ring slippage reactions, cyclometallation reaction.

**UNIT-II**

**13h**

**Organometallic compounds of main group elements-** General trends, structure and bonding in Li and Al alkyls.

**Fluxional behaviour in organometallic complexes:** Fluxionality and dynamic equilibria in complexes containing CO,  $\eta^2$ -olefin  $\eta^3$ -allyl and dienyl complexes.

**Organometallic compounds in organic synthesis:** Green rules, synthesis and use of Zinc dialkyls, Collman's reagent, organomercuric and chromium carbonyls in organic synthesis, Heck reaction, hydrozirconation.

**UNIT-III**

**A. Isoelectronic and isolobal analogy.**

**13h**

**B. Catalysis-** Basic principles, industrial requirements of catalysts.

**Homogeneous catalysis:**

Hydrogenation-Wilkinson catalyst, Crabtree's catalyst,  $\text{RuHCl}(\text{PPh}_3)_3$ .

Asymmetric hydrogenation of methyl(Z)- $\alpha$ -acetamidocinnamate, synthesis of L-DOPA, chiral phosphines; Hydrosilation- Chalk-Harrod mechanism:

Hydrocyanation of buta-1,3-diene; synthesis of adiponitrile.

Hydroformylation- Cobalt and modified catalysts, Rh catalysts.

**UNIT-IV****13h**

Wacker process- acetaldehyde from ethylene; Monsanto acetic acid process, Cativa process, Tennessee Eastmann process- Acetic anhydride from methyl acetate. Olefin metathesis-mechanism, ring opening metathesis, ring closing metathesis, cross metathesis; water gas shift reaction; Oligomerization- Shell High Olefin process; alkene isomerisation.

**Heterogeneous catalysis:**

Fischer Tropsch Process; Ziegler Natta Polymerization- syndiotactic, isotactic polymers, living polymerization; ammonia synthesis-Haber-Bosch process; Anchored catalysis- merits, polymer and metal oxides as supports; catalytic converters.

**SUGGESTED BOOKS**

1. Organometallic Chemistry; R. C. Mehrotra and A. Singh; New age international, 2<sup>nd</sup> edition, 2000.
2. The organometallic chemistry of transition metals; R. H. Crabtree; John Wiley, 3<sup>rd</sup> edition, 2001.
3. Organometallic Chemistry, ch. Elschewbroich and Slazer, VCH, 2<sup>nd</sup> edition 1992.
4. Organometallics; Vol 1 & 2; M. Bochmann, Oxford Chemistry Primers, Oxford University Press, 1994.
5. Catalytic chemistry; B. C. Gates; John Wiley and sons, 1992.
6. Applied Organometallic chemistry and catalysis; Robin whyman, Oxford University Primers, 2001.
7. Basic Organometallic chemistry; B. D. Gupta and A. J. Elias, Universities Press, 2<sup>nd</sup> edition 2013.
8. Heterogeneous catalysis; D. K. Chakraborty and B. Viswanathan, New Age International, 2000.

**Ch 403 IC: CHEMISTRY OF MATERIALS****52 Hours****UNIT-I****13h**

**Preparative Techniques:** Principles of solid state synthesis- ceramic methods, solid solution and compound precursors (nitrates, carbonates, hydroxides, cyanides and organometallics), sol-gel, spray pyrolysis, combustion, hydrothermal, electrosynthetic

**New Materials**

Fullerenes and fullerides – structure, synthesis, functionalization approaches, conducting properties of fullerides. applications.

NASICON and alumina – structure and conducting properties.

High- $T_c$  Oxides - structure, perovskite A & B, structure and synthesis of La, Sr and Ba cuprates, applications..

Conducting polymers - PA, PPP, PPS, PPY-mechanism of conduction and applications.

## UNIT-II

13 h

**Nanomaterials:** Classification types of carbon nano tubes synthesis, functionalization characterization and applications.

Principles of self-assembly: surfactant solutions, importance of non-covalent forces, the hydrophobic effect, co-operativity, statistical mechanics of one-dimensional self-assembly. Preparation of nanoscale materials: Precipitation, mechanical milling, colloidal routes, self assembly: chemical vapour deposition, sputtering, evaporation.

Synthesis, characterization and applications of nanoparticles, nano wires and nanotubes. Elemental nanoparticles: Pure, Gold, Silicon, Silver, Cobalt, Oxide nanoparticles: Silica, Zinc oxide, Iron oxide, Alumina.

## UNIT-III

13 h

**Intercalation Compounds:** Intercalation reactions - layered structure-graphite interlayer compounds (GILC), staging of graphite, TaS<sub>2</sub>, Microporous materials – zeolites and zeolitic materials, AlPO<sub>4</sub>- GaPO<sub>4</sub>.

### **Fibres and Composites**

Synthetic inorganic polymers- zirconia and other fibre Classification, microscopic composites, dispersion strengthened, particle reinforced, Fibre-glass reinforced composites, metal-matrix, plastic-matrix composites, hybrid composites.

## UNIT-IV

13 h

**Amorphous Materials:** Crystalline versus amorphous solids, glass formation, Preparation techniques- meltspinning, sputtering, ion implantation, Structural models of amorphous materials, Properties of metglasses - mechanical, electronic and magnetic properties.

**Liquid Crystals:** Mesomorphic behaviour, classification, examples - thermotropic and lyotropic liquid crystals Calamitic, nematic phase A, B, smectic phase, chiral nematic phase and optical Properties of liquid crystals. Applications with special reference to display systems

## **SUGGESTED BOOKS**

1. Encyclopedia of Nanomaterials and Nanotechnology Hari Singh Nalwa.  
<http://www.aspbs.com/enn.html>
2. Nanostructured Materials: Processing, Properties and Applications, ed. C.C.Koch, William Andrew Publishing, New York, 2002.
3. Nanomaterials: Synthesis, properties and applications, Ed. By A.S.Edelstein and R.C. Cammarata, Inst. of Physics, UK 1966.
4. Science of Engineering Materials, C.M. Srivastava and C. Srinivasan, Wiley-Eastern Ltd. (1991).
5. Solid State Chemistry and its Applications, A.R. West, John Wiley & Sons.(1989).
6. Material Science and Engineering. W.D. Callister, John Wiley and Sons Inc. (1985).
7. Nanotubes and Nano wires CNR Rao, & A Govindaraj, RSC, London 2005.
8. NANO: The essentials T. Pradeep, McGraw-Hill, 2008.
9. Liquid Crystals, Nature's delicate phase of matter, Peter J Collings, Princeton University Press, 2002
10. Nanochemistry, A chemical approach to Nanomaterials, Geoffrey A Ozin and Andre C

## Ch-404 IC/ PC: INORGANIC SPECTROSCOPY

(Common to Inorganic and Physical Chemistry)

52 Hours

### UNIT-I

13h

#### **Vibrational spectroscopy**

Vibrational spectra of diatomic, linear and bent triatomic, AB<sub>3</sub>, AB<sub>4</sub>, AB<sub>5</sub> and AB<sub>6</sub> molecules, spectra of metal complexes: Ammine, amido, Nitro, Nitrito, lattice water, aquo and hydroxo, carbonato, nitrate, sulphato and other acido complexes, cyano and nitrile complexes, cyanato and thiocyanato complexes, mono and multinuclear carbonyl complexes, nitrosyls, phosphines and arsines, ambidentate ligands, ethylenediamine and diketonato complexes.

#### **Raman spectroscopy**

Resonance Raman Spectroscopy, Nonlinear Raman effects-Stimulated, hyper and inverse types, coherent anti-stokes raman scattering (CARS) Lasers and their use in Raman spectroscopy. Resonance Raman spectrum of K<sub>2</sub>CrO<sub>4</sub> and complexes with peroxide linkage.

### UNIT-II

13h

#### **Photoelectron spectroscopy**

Basic principles- photoelectric effect, Koopman's theorem, XPS and UPS, spin-orbit coupling in core level spectra, applications of core level spectra-ESCA, chemical shift, Valence level spectra- n,  $\sigma$  and  $\pi$  bands, Auger electron spectroscopy and applications, Electron energy loss spectroscopy- basic principles and applications  
Applications to the study of solids.

#### **Mossbauer spectroscopy**

Basic principles, isomer shift, quadrupole splitting and magnetic hyperfine interactions, application to the study of bonding and structures of Fe<sup>2+</sup> and Fe<sup>3+</sup> compounds, Sn<sup>2+</sup> and Sn<sup>4+</sup> compounds

### UNIT-III

13h

#### **Electron spin resonance spectroscopy**

Basic principles, the position of ESR absorption, significance of 'g' factor, determination of 'g' factor. Electron-nucleus coupling (Hyperfine splitting). ESR spectrometer, electron-electron coupling, double resonance in ESR, ENDOR, ELDOR.

Interpretation of ESR spectra and structure elucidation of organic radicals using ESR spectroscopy. Spin density and Mc Connell relationship. Spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, zero/non-zero field splitting, Kramer's degeneracy, application to transition metal complexes (having one to five unpaired electrons) including

biological molecules and inorganic free radicals such as  $\text{PH}_2$ ,  $\text{F}_2$  and  $\text{BH}_3$ .

### **X-ray absorption spectroscopy**

Near edge measurements and EXAFS

## **UNIT-IV**

### **NMR spectroscopy of inorganic molecules**

13h

Proton NMR spectra of metal hydride complexes

NMR spectra of nuclei other than hydrogen:  $^{19}\text{F}$ ,  $^{31}\text{P}$ ,  $^{11}\text{B}$  NMR spectra of simple compounds,

Proton/hydride interactions with  $^{103}\text{Rh}$ ,  $^{183}\text{W}$ ,  $^{195}\text{Pt}$  and  $^{207}\text{Pb}$  in metal complexes/organometallic compounds,

Solid State NMR.

### **NQR spectroscopy**

NQR isotopes, electric field gradients, Nuclear Quadrupole coupling constants, Experimental techniques and applications

### **SUGGESTED BOOKS**

1. Physical methods in Inorganic Chemistry, R.S. Drago, Affiliated East West Press Pvt. Ltd., New Delhi 1965.
2. Infrared spectra of Inorganic and Coordination Compounds, K. Nakamoto, Wiley Interscience, New York 1970.
3. Vibrational Spectroscopy: Theory and Applications, D.N. Sathyanarayana, New Age International Publishers, New Delhi 2000.
4. Electronic Absorption Spectroscopy and Related Techniques, D.N. Sathyanarayana, Universities Press, Bangalore 2001.
5. Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR, D.N. Sathyanarayana, I.K. International Publishing House Pvt.Ltd., New Delhi 2009.

## **INORGANIC CHEMISTRY PRACTICALS**

(4 days a week, 4 hours a day)

### **Ch 405 IC: Inorganic Quantitative Analysis-I**

1. Determination of % purity of nitrite by chloramine-T.
2. Determination of % cobalt in  $[\text{Co}(\text{NH}_3)_6]\text{Cl}_3$ .
3. Determination of % purity of sulphate by EDTA.
4. Determination of sulphate using benzidine hydrochloride.
5. Microvolumetric estimation of chloride by Volhard's method.
6. Determination of %  $\text{NH}_3$  in  $[\text{Co}(\text{NH}_3)_6]\text{Cl}_3$  by microkjeldahl method.
7. Preparation of tetraamminecopper(II) sulphate hydrate  $\text{Cu}(\text{NH}_3)_4\text{SO}_4 \cdot \text{H}_2\text{O}$ .
8. Preparation of bis(ethylenediamine)copper(II) sulphate  $[\text{Cu}(\text{en})_2]\text{SO}_4$ .
9. Preparation of cis-bis(glycinato)copper(II) monohydrate  $\text{cis}-[\text{Cu}(\text{glycine})_2] \cdot \text{H}_2\text{O}$ .

### **Ch 406 IC: Inorganic Quantitative Analysis-II**

1. Determination of copper as copper salicylaloximate complex.
2. Determination of % chloride in  $[\text{Co}(\text{NH}_3)_6]\text{Cl}_3$  by gravimetry / ion exchange method.
3. Determination of Mg as  $\text{Mg}(\text{NH}_4)\text{PO}_4$  and  $\text{Mg}_2\text{P}_2\text{O}_7$ .

4. Estimation of metal acetate using perchloric acid in glacial acetic acid medium.
5. Estimation of Fe(III) by solvent extraction.
6. Separation of mixture of metal ions by paper chromatography (Cu, Ni and Co).
7. Analysis of hindalium alloy.
8. Analysis of woods alloy.

#### Ch 407 IC: Instrumental Methods-I

1. Spectrophotometric determination of  $\text{Fe}^{3+}$  by using o-phenanthroline.
2. Spectrophotometric determination of  $\text{Fe}^{3+}$  by using thiocyanate.
3. Spectrophotometric determination of  $\text{Ni}^{2+}$  using DMG.
4. Determination of Cu by spectrophotometry.
5. Determination of  $\lambda_{\text{max}}$ ,  $\Delta_0$  and assignment of UV-Visible spectrum of  $\text{Co}(\text{NH}_3)_6\text{Cl}_3$  complex.
6. Assignment of electronic spectra of Cu complexes of  $\text{NH}_3$ , ethylenediamine glycine (synthesized in 405) and correlation of  $\lambda_{\text{max}}$  with ligand field strength.
7. Spectrophotometric determination of aluminium using aluminon reagent.
8. Spectrophotometric determination of Cr(VI) and Mn(VII) in a mixture of  $\text{K}_2\text{Cr}_2\text{O}_7$  and  $\text{KMnO}_4$ .

#### Ch 408 Instrumental Methods-II

1. Flame photometric determination of Na.
2. Flame photometric determination of K.
3. Determination of cell constant and molar conductivity of 1:1, 1:2 and 1:3 complexes.
4. Electrogravimetric estimation of copper.
5. Determination of formation constant of ferrisalicylate complex.
6. Determination of composition of Fe-1,10 phenanthroline complex by Job's method.
7. Determination of magnetic susceptibility of  $\text{Hg}[\text{Co}(\text{SCN})_4]$ .
8. Thermogravimetric analysis of  $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$ .

#### Suggested Books:

1. A text book of Quantitative Analysis; A. I. Vogel; ELBS, 1962.
2. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Von Nostrand Reinhold Co., London 1972.
3. Experimental Inorganic Chemistry; G. Palmer, Cambridge University Press, 1954.
4. Hand Book of preparative inorganic chemistry, Vols I and II; G. Brauer, Academic Press, 1963.
5. Non- aqueous titrations; W. Huber; Academic Press, 1967.
6. Experimental Methods in inorganic chemistry; T. Tanaka and S. L. Suib, Prentice Hall, 1999.
7. Experiments in Chemistry; D. V. Jahagirdar, Himalayan Pub House, 2003.

**THIRD SEMESTER**  
**ORGANIC CHEMISTRY SPECIALISATION**  
**Ch-301 OC: ORGANIC REACTION MECHANISMS**

52 hours

**UNIT-I**

13h

**Aliphatic nucleophilic and electrophilic substitution reactions**

*Nucleophilic substitution reactions:*

Substitution at allylic carbon (allylic rearrangement), at a trigonal carbon (hydrolysis of esters and amides, use of DCC in the formation of anhydrides), substitution at a vinylic carbon.

Neighboring group participation and S<sub>N</sub>i reactions.

*Electrophilic substitution reactions:*

SE<sub>2</sub>, SE<sub>1</sub> and SE<sub>i</sub> mechanisms. Hydrogen exchange, migration of double bonds, α-halogenation of aldehydes, ketones and acids. Aliphatic diazonium coupling, nitrosation at carbon bearing active hydrogens, diazo transfer reaction, carbene and nitrene insertion, decarboxylation of aliphatic acids, haloform reaction, Haller-Bauer reaction.

**UNIT-II**

13h

**Photochemistry**

Physical and Chemical processes, Jablonski diagram. Photosensitization, quantum efficiency, quantum and chemical yields.

*Photochemistry of functional groups:*

i) *Olefins:* *Cis-trans* isomerism, [2 + 2]-cycloaddition, rearrangements. Reaction of conjugated olefins; di-π-methane rearrangements (including oxa- and aza- di-π-methane rearrangements).

ii) *Ketones:* Excited state of C=O. Norrish type-I and type-II cleavages. Paterno-Buchi reaction. α,β-unsaturated ketones. [2+2] addition. Rearrangement of cyclohexadienones (application in the synthesis of some important natural products).

iii) *Aromatic compounds:* Photorearrangement of benzene and its derivatives, cycloaddition of benzene.

iv) *Photochemical oxidations and reductions:* Cycloaddition of singlet molecular oxygen {[2+2], [4+2]-additions}. Oxidative coupling of aromatic compounds, photoreduction by hydrogen abstraction.

**UNIT-III**

13h

**Pericyclic reactions**

Molecular orbital symmetry, Woodward-Hoffmann correlation diagrams. FMO and PMO approaches. Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system.

*Electrocyclic reactions:* conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems.

*Cycloadditions:* antarafacial and suprafacial additions, [πm<sub>s</sub> + πn<sub>a</sub>] and [πm<sub>s</sub> + πn<sub>s</sub>]-cycloadditions. [ω2<sub>a</sub> + π2<sub>s</sub>] and [π4<sub>s</sub> + ω2<sub>s</sub>]-cheletropic reactions.

Regio, enantio- and endo- selectivities in Diels-Alder reactions. Hetero Diels-Alder reaction.

*Sigmatropic rearrangements:* suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties. [*i, j*]- sigmatropic rearrangements (including Walk, Claisen, Cope, oxy and aza-Cope rearrangements).

#### **UNIT-IV**

13h

##### **Free-radical chemistry**

Generation of free-radicals: Thermal homolysis of peroxides, peresters and azo compounds, photochemical methods.

Free radical reactions: Free-radical mechanisms in general. Free-radical substitution mechanisms. Mechanisms at an aromatic substrate. Neighboring group assistance in free-radical reactions. Reactivity for aliphatic substrates, reactivity at a bridgehead, reactivity in aromatic substrates, reactivity in the attacking radical. Halogenation at an alkyl carbon and an allylic carbon, hydroxylation at an aliphatic carbon, hydroxylation at an aromatic carbon, oxidation of aldehydes to carboxylic acids, formation of hydroperoxides and peroxides, Gomberg-Bachmann reaction, Meerwein arylation, Sandmeyer reaction, Kolbe reaction and Hunsdiecker reaction.

##### **Biochemical mechanisms**

Introduction. The mechanistic role of the following in living systems.

- i). Thiamine pyrophosphate (TPP) in decarboxylation of  $\alpha$ -ketoacids and in the formation of  $\alpha$ -ketols.
- ii). Pyridoxal phosphate (PLP) in transamination, decarboxylation, dealdolisation and elimination reactions of amino acids.
- iii). Lipoic acid in the transfer of acyl group reactions.
- iv). Coenzyme A (CoASH) in the transfer of acyl group.
- v). Biotin and Vitamin K<sub>H2</sub> coenzyme in carboxylation reactions.
- vi). Tetrahydrofolic acid (H<sub>4</sub>F) in one-carbon transfer reactions.
- vii). Vitamin B<sub>12</sub> coenzymes in molecular rearrangement reactions and in the synthesis of methionine and methane.
- viii). Nicotinamide and Flavin coenzymes in biological redox reactions

#### **SUGGESTED BOOKS**

1. March's Advanced Organic Chemistry – Reactions, Mechanisms and Structure, M B Smith and J March, 8<sup>th</sup> Edition, John Wiley, 2019.
2. Modern molecular photochemistry of organic molecules, N J Turro, V Ramamurthy, J C Scaiano, Viva Books, New Delhi – 2017.
3. Textbook of pericyclic reactions – concept and application, K C Majumdar and P Biswas, Medtech, New Delhi – 2015
4. Organic Chemistry II edition, J Clayden, N Greeves and S Warren, Oxford Univ. Press, Oxford, 2012.
5. Frontier orbital and symmetry controlled pericyclic reactions, R K Kar, Books and Allied, Kolkata, 2010.
6. Advanced Organic Chemistry – Reactions, Mechanism and Structure, Jerry March, John Wiley, 2008.
7. Stereochemistry at a glance, J Eames and J M Peach, Blackwell, Oxford, 2003.
8. Advanced Organic Chemistry – Reaction Mechanisms, R. Bruckner, Harcourt/Academic Press, London, 2002.
9. Stereochemistry of Organic Compounds: Principles and Applications, D Nasipuri, New- Age

International, 1999.

10. Understanding organic reaction mechanisms, A. Jacob, Cambridge Univ. Press, 1997.
11. Radicals in organic synthesis, B. Giese, Pergamon Press, 1986.
12. Introduction to organic chemistry A. Streitwieser, Jr and C. H. Heathcock, Macmillan, 1985.
13. Stereoelectronic effects in organic chemistry, P. Deslongchamps, 1<sup>st</sup> Edn. Pergamon Press, 1983.
14. Frontier orbitals and organic chemical reactions, Oxford University Press primers, I Fleming, John Wiley, 1980.
15. Physical and mechanistic organic chemistry, R.A.Y. Jones, 1<sup>st</sup> Edn. Cambridge Univ. Press, 1979.
16. Mechanisms of molecular migrations, Vols I and II, B. S. Thiagarajan, 1<sup>st</sup> Edn. Pergamon Press, Oxford, 1979.
17. P. J. Garratt in Comprehensive organic chemistry, D. Barton and W. D. Ollis, 1<sup>st</sup> Edn. Pergamon Press, Oxford, 1979.
18. Organic photochemistry, J. M. Coxon and B. Halton, Cambridge Univ. Press, London, 1974.
19. Orbital symmetry, R. E. Lehr and A. P. Marchand, Academic Press, 1972.
20. Molecular reactions and photochemistry, C. H. Depuy and D. S. Chapman, 1<sup>st</sup> Edn. Prentice-hall India, New Delhi, 1972.
21. Molecular orbital theory for organic chemistry, A. Streitwieser, 1<sup>st</sup> Ed. Wiley & Sons, NY, 1969
22. Biochemistry, G. Zubey, Macmillan, NY, 1998.
23. Biochemistry, D. Voet and J. G. Voet, John Wiley & Sons, 2010.
24. Principles of Biochemistry, A. L. Lehninger, D. L. Nelson & M. M. Cox, Worth Publishers, NY, 2013.
25. Biochemistry illustrated, P N Campbell, m A D Smith, 3<sup>rd</sup> edition, Churchill Livingstone, Edinburgh, 1994.

### Ch-302 OC: ORGANIC SYNTHESIS

52Hours

#### UNIT - I

13h

##### **C-C and C-N bond forming reactions**

Darzen's reaction, Use of acetylides in C-C bond formation reactions. Acid-catalyzed self condensation of olefins, Prins reaction, Shapiro reaction, Dieckmann cyclization, Robinson annulations, Hofmann-Loeffler-Freytag reaction. Hofmann-Martius reaction. Acyloin condensation. Houben-Hoesch reaction.

Stork-enamine synthesis. Meyer synthesis. Use of nucleophilic nitrogen and electrophilic carbon (NH<sub>3</sub>, amines and nitrite as nucleophiles in substitution, NH<sub>3</sub> and amines in addition to ketones and aldehydes) and electrophilic nitrogen and nucleophilic carbon (nitration, nitrosation) for the bond formation reactions (including Chichibabin reaction, Skraup synthesis, Mitsunobu reaction, N-Nitroaromatic amine rearrangement, Fisher-Hepp reaction. Japp-Klingemann reaction).

#### UNIT-II

13h

##### **Reagents in organic synthesis and functional group transformation**

NBS, LDA, DCC, DDQ, Corey-Chaykovsky reagent, Raney-Nickel, diazomethane, TMS-chloride, 1,3-Dithiane (reactivity and umpolung) and PPA. Woodward and Prevost hydroxylation.

##### **Oxidations**

Cr (VI) oxidants, Mn (VII) oxidants, OsO<sub>4</sub>, SeO<sub>2</sub>, Pb(OAc)<sub>4</sub>, HIO<sub>4</sub>, Ag<sub>2</sub>O, DMSO, Ozone, peroxides and peracids - as oxidizing agents. Oppenauer and Dess-Martin oxidation.

### UNIT-III

#### **Reductions**

13h

Complex metal hydrides, Birch, Clemmensen and diimide reduction. Catalytic hydrogenation (homogeneous and heterogeneous). Organoboranes as reducing agents. Wolf-Kishner and Meerwein-Ponndorf-Verley reduction. McMurry, Pummer, Willgerdot, Corey-Bakshi-Shibata and Tishchenko reactions.

### UNIT-IV

13h

#### **Asymmetric Synthesis**

'*ee*' and methods of determination of '*ee*'.

*Stereoselectivity*: classification, terminology and principle. Asymmetric synthesis and asymmetric induction.

Double diastereoselection and double asymmetric induction.

*Acyclic stereoselection*: Addition of nucleophiles to carbonyl compounds (1,2- 1,3- and 1,4-asymmetric induction). Asymmetric aldol condensation. Addition of allylmetal and allylboranes to carbonyl group.

*Diastereoselection in cyclic systems*: Nucleophilic addition to cyclic ketones (formation of axial and equatorial alcohols, catalytic hydrogenation, alkylation, diastereoselective oxidations and stereoselective cyclization of polyenes).

*Enantioselective synthesis*: Reduction with chiral hydride donors [(S)-PBMgCl, (-)-'BOAlCl<sub>2</sub>, alpine-borane, (S)-BINAL-H, (R,R)-DIOP, and (S,S)-CHIRAPHOS].

Enantioselective alkylation of ketones *via* hydrazones. Enantioselective alkylation with chiral PTC. Enantioselective Michael addition. Enantioselective intramolecular aldol condensation. Use of (+)- and (-)- DET in asymmetric epoxidation. Polymer-bound chiral catalysts in asymmetric induction. Asymmetric amplification.

#### **SUGGESTED BOOKS**

1. March's Advanced Organic Chemistry – Reactions, Mechanisms and Structure, M B Smith and J March, 8<sup>th</sup> edition, John Wiley, 2019.
2. Essential reagents for organic synthesis, P L Fuchs, A B Charette, T Rovis, Wiley, NY, 2016.
3. Modern methods of organic synthesis, 4<sup>th</sup> edition, W. Carruthers and I Coldham, Cambridge Univ. Press, Cambridge, 2014.
4. Name reactions, 5<sup>th</sup> edition, J J Li, Springer, 2014.
5. Asymmetric synthesis II, more methods and applications, M Christman, S. Brase, Wiley - VCH, 2013.
6. Organic chemistry Vol. II, I. L. Finar 6<sup>th</sup> edition Pearson, New Delhi - 2012.
7. Asymmetric synthesis: the essentials, 2<sup>nd</sup> edition, M Christman, S. Brase – Eds., Wiley - VCH, 2007.
8. Organic reaction mechanisms, 3<sup>rd</sup> Edn., V. K. Ahluwalia and R. K. Prashar, Narosa, New Delhi, 2005.
9. Name reactions and reagents in organic synthesis, 2<sup>nd</sup> edition, B P Mundy, M G Ellerd, F G Favalaro Jr. Wiley, NY – 2005.
10. M B Smith, Collective index for volumes 1-22 of Fiesers reagents for organic synthesis, Wiley-Interscience, NY, 2005.

11. Oxidation and reductions in organic synthesis, T J Donohoe, Oxford University Press primer, Oxford, 2000.
12. Understanding organic reaction mechanisms, A. Jacob, Cambridge Univ Press, 1997.
13. Introduction to organic chemistry, A. Streitwieser, Jr and C. H. Heathcock, Macmillan, 1985.
14. Comprehensive organic chemistry, D. Barton and W. D. Wallis, Pergamon Press, Oxford, 1983.
15. Physical and mechanistic organic chemistry, R. A.Y. Jones, 1<sup>st</sup> Edn. Cambridge University Press, 1979.
16. Modern synthetic reactions, H. O. House, W. A. Benjamin, California, 2<sup>nd</sup> edition. 1972.
17. Mechanisms of molecular migration, Vols I & II, B.S. Thyagarajan, Pergamon Press, Oxford, 1979.
18. Organic synthesis, R.E.Ireland, Prentice-hall India, New Delhi, 1975.
19. Oxidation and reduction of organic compounds, K L Rinehart Jr. Prentice – Hall, 1973.
20. Fiesers' reagents for organic synthesis, Volumes 1-22, 1967-2000

**Ch-303 IC/OC/PC: ORGANIC SPECTROSCOPY**  
(Common to Inorganic/ Organic/ Physical chemistry)

**52 Hours**

**UNIT-I**

**13h**

**Ultraviolet/ visible spectroscopy**

Instrumentation. Classification of electronic transitions. Substituent and solvent effects.

UV spectral study of alkenes, polyenes,  $\alpha,\beta$ -unsaturated carbonyl and aromatic compounds. Empirical rules for calculating  $\lambda_{\max}$ .

**Vibrational Spectroscopy: Infrared and Raman spectroscopy**

Instrumentation. Sampling techniques, Group frequencies, factors affecting group frequencies, Bond order, Mass effect, Conjugation, Inductive, resonance, steric effects. Intramolecular interactions. Application of IR in the study of H-bonding, stereoisomerism and tautomerism. Complementarity of IR and Raman. Identification of the following organic compounds by IR: alkanes, alkenes, alkynes, aromatic compounds, aldehydes, ketones, alcohols, acids, acid chlorides, amides, amines, esters, halides and nitro compounds etc. Problems using UV and IR.

**UNIT-II**

**13h**

**Nuclear magnetic resonance spectroscopy-I**

Introduction, Magnetic properties of nuclei- Resonance condition. Nuclear spin, population of nuclear spin levels and NMR isotopes, Relaxation methods. Instrumentation and sample handling, FT-NMR.

Chemical shift. Mechanism of shielding and deshielding in Alkanes, Alkyl halides, Alkenes, Aromatic compounds, Carbonyl compounds and Annulenes. Pascal's triangle-low and high resolution, spectrum of ethanol. Karplus Curve, Diamagnetic and paramagnetic effects and magnetic anisotropy. Equivalence of protons-chemical and magnetic equivalence. Spin-systems: First order and second order coupling of AB systems, Simplifications of complex spectras.

Problems.

Spin-spin interactions: AX, AX<sub>2</sub>, AX<sub>3</sub>, AMX, AB types. Vicinal, geminal and long range coupling-Spin decoupling. Chemical shift reagents and deuterium exchange. Stereochemistry and hindered rotations. Temperature effects.

### UNIT-III

13h

#### **Nuclear magnetic resonance spectroscopy-II**

CIDNP, Nuclear Overhauser effect (NOE). Factors influencing coupling constants and Relative intensities. Protons attached to elements other than carbon.

<sup>13</sup>C NMR Spectroscopy: Range and factors affecting chemical shifts of alkanes, alkyl halides, alkenes, alcohols, ethers, alkynes, carbonyl compounds and aromatics..

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

Explanation of the principle, applications to structure elucidation and stereochemistry of simple organic molecules.

Dynamic NMR.

NMR spectroscopy of other nuclei with spin I = ½. Introduction to <sup>15</sup>N, <sup>19</sup>F, <sup>29</sup>Si and <sup>31</sup>P NMR spectroscopies.

### UNIT-IV

13h

#### **Mass spectrometry and Composite Problems:**

Basic principles-instrumentation – ion production-ion analysis-magnetic sector instruments Quadrupole mass spectrometers. Time of flight mass spectrometers-ion cyclotron resonance spectrometers- Mass spectrum-molecular ion-types of ions in mass spectra and effects of isotopes on mass spectra. Methods of ionization, EI, FAB MALDI and ESI methods. Fragmentation of alkanes, alkenes, aromatics, alkyl halides, alcohols, aldehydes, ketones, acids, esters, ethers, amines, nitro and halo compounds peptides, Nitrogen rule, Factors affecting cleavage patterns. McLafferty rearrangement. Determination of molecular formula. Problems.

Use of HRMS to determine exact molecular formulae of compounds.

Application of UV, IR, NMR and MS methods and chemical reactions in the structure elucidation of organic compounds – composite problems.

### **SUGGESTED BOOKS**

1. Spectroscopic methods in organic chemistry, 7<sup>th</sup> edition, D Williams and I Fleming, Springer International Publishing, Berlin – 2019
2. Fundamentals of molecular spectroscopy 5<sup>th</sup> edition, C N Banwell, E M McCash, H K Choudhury, Tata McGraw Hill, New Delhi - 2015
3. Spectrometric identification of organic compounds, R. M. Silverstein, F X Webster, D J Kiemle and D L Bryce, 8<sup>th</sup> Wiley student edition, New Delhi, 2015.
4. Organic spectroscopy, W. Kemp, Macmillan, London, 2011.
5. Introduction to spectroscopy, 4<sup>th</sup> edition, D. L. Pavia, G. M. Laupman and G. S. Kriz, Harcourt College Publishers, 2009.
6. Structure determination of organic compounds E Pretsch, P Buhlmann and M Badertscher, Springer-Verlag, Berlin – 2009.
7. Spectroscopic methods in organic chemistry, M Hesse, H Meier, B Zeeh, 2<sup>nd</sup> edition, Thieme, Stuttgart, 2008.

8. Organic Spectroscopy, LDS Yadav, Springer/Kluwer, 2005.
9. Organic Spectroscopic Analysis, R J Anderson, D J Bendell, P W Groundwater, RSC, Cambridge, 2004.
10. Mass spectrometry a foundation course, K Downard, RSC, Cambridge, 2004.
11. Structural analysis of organic compounds by combined application of spectroscopic studies, J T Clerc, E Pretsch, J Seibl, Elsevier, Amsterdam, 2001.
12. Biomolecular NMR Spectroscopy, J N S Evans, Oxford University, Oxford, 1995.
13. Modern NMR techniques and their Applications, Ed. A I Popov, Marcel Dekker, 1991.
14. Instrumental methods of analysis, H. H. Willard, L. L. Merritt, J. A. Dean and F.A. Settle, 7<sup>th</sup> edition, CBS Publishers and Distributors, 1989
15. Organic mass spectroscopy, K. R. Dass & E. P. James, IBH New Delhi, 1976.
16. The IR Spectra of complex molecules, Vols. I and II, L J Bellamy, Chapman and Hall, London, 1975.
17. Mass spectrometry of organic compounds, H. Budzkiewicz, Djerassi C. and D. H. Williams, Holden-Day New York, 1975.
18. Interpretation of organic mass spectra, F W McLafferty, W A Benjamin, London, 1973.
19. Organic spectroscopy, P. Laszlo and P. Stang, Harper & Row, New York, 1971.
20. Applications of absorption spectroscopy to organic compounds, J. R. Dyer, Prentice-Hall, New Delhi, 1969.
21. Interpretation of the UV spectra of natural products, A.I. Scott, Pergamon Press, Oxford, 1964.

**Ch-304-[OPEN ELECTIVE, NON-CHEMISTRY PAPER]**

**OPEN ELECTIVE FOR NON-CHEMISTRY STUDENTS**  
**Ch-304 OE: CHEMISTRY IN DAILY LIFE**

**52 Hours**

**UNIT-I**

**13h**

**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, disulphites,

**Artificial sweeteners:** aspartame, saccharin, dulcin, sucralose and sodium cyclamate.

**Flavours:** Vanillin, alkyl esters (fruit flavours) and monosodium glutamate.

**Artificial food colorants:** Coal tar dyes and non-permitted colours and metallic salts. Analysis of pesticide residues in food.

**Paints & Pigments:** White pigments (white lead, ZnO, lithopone, TiO<sub>2</sub>). Blue, red, yellow and green pigments. Paints and distempers: Requirement of a good paint. Emulsion, latex; luminescent paints. Fire retardant paints and enamels, lacquers. solvents and thinners for paints.

**Dyes:** Colour and constitution (electronic concept). Classification of dyes. Methods of applying dyes to the fabrics. A general study of azo dyes, Mordant brown, Congo red and methyl orange.

**UNIT II**

**13h**

**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.

**Composition of soil** – inorganic and organic components in soil-micro and macronutrients.

**Fertilisers:** Classification of Fertilizers- Straight Fertilizers, Compound/Complex Fertilizers, Fertilizer Mixtures. Manufacture and general properties of Fertilizer products- Urea and DAP.

**UNIT-III**

**13h**

**Carbohydrates:** Structure, function and Chemistry of some important mono and disaccharides.

**Vitamins:** Classification and Nomenclature. Sources, deficiency diseases and structures of Vitamin A, Vitamin B, Vitamin C, Vitamin D, Vitamin E & Vitamin K.

**Drugs:** Classification and nomenclature.

Structure and function of: *Analgesics* – aspirin, paracetamol;

*Anthelmintic drug:* mebendazole;

*Antiallergic drug:* Chlorpheniramine maleate,

*Antibiotics:* Penicillin V, Chloramycetin, Streptomycin.

*Anti-inflammatory agent:* Oxyphenbutazone,

*Antimalarials:* Primaquine phosphate & Chloroquine.

**Oils and fats:** Composition of edible oils, detection of purity, rancidity of fats and oil. Tests for adulterants like argemone oil and mineral oils.

**Soaps & Detergents:** Structures and methods of use of soaps and detergents.

## UNIT IV

13h

**Chemical Thermodynamics:** Concept of fugacity and free energy, Activity and activity coefficient, spontaneity of processes- entropy and free energy changes. Partial molar quantities, colligative properties, Le-Chatelier principle, phase equilibria. Enzyme catalysed reactions.

**Principles of Reactivity:** Basis kinetic concepts, rates of simple and complex chemical reactions, empirical rate equations. Temperature dependence of rates and activation parameters. Branched chain reactions – explosion limits. Oscillatory reactions.

**Corrosion:** Types and prevention, corrosion failure and analysis

**Chemical energy system** and limitations, principles and applications of primary & secondary batteries and fuel cell. Basics of solar energy, future energy storers.

**Polymers :** Types and classification of polymers. Source and general characteristics of natural and synthetic polymers. Typical examples of polymers used as plastics, in textiles, in electronic and automobile components, in the medical and aerospace materials. Problems of plastic waste management. Strategies for the development of environment friendly polymers.

### **SUGGESTED BOOKS**

1. B. K. Sharma: introduction to Industrial Chemistry, Goel Publishing, Meerut (1998)
2. Medicinal Chemistry by Ashtoush Kar.
3. Drugs and Pharmaceutical Sciences Series, Marcel Dekker, Vol. II, INC, New York.
4. Analysis of Foods – H.E. Cox: 13. Chemical Analysis of Foods – H.E.Cox and Pearson.
5. Foods: Facts and Principles. N. Shakuntala Many and S. Swamy, 4<sup>th</sup> ed. New Age International (1998)
6. Physical Chemistry – P I Atkins and J. de Paula – 7<sup>th</sup> Ed. 2002, Oxford University Press.
7. Handbook on Fertilizer Technology by Swaminathan and Goswamy, 6<sup>th</sup> ed. 2001, FAI.
8. Organic Chemistry by I. L. Finar, Vol. 1 & 2.
9. Polymer Science and Technology, J. R. Fried (Prentice Hall).

*and*  
**Ch-305, 306, 307 and 308 OC Practicals**  
**Inorganic, Organic, Physical ~~and Analytical~~ Chemistry practicals (I Semester Syllabus) (4 days a week, 4 hours a day)**

**FOURTH SEMESTER**  
**ORGANIC CHEMISTRY SPECIALIZATION**  
**Ch-401 OC: ADVANCED STEREOCHEMISTRY AND RETROSYNTHETIC**  
**ANALYSIS**

**52 Hours**

**UNIT-I**

**13h**

**Advanced Stereochemistry – I**

**Optical activity in the absence of chiral atoms**

Chirality in biphenyls, adamantanes, ansa compounds, cyclophanes, *trans*-cyclooctene, catenanes, rotaxanes and helicenes. Assignment of R, S- configuration to these classes of compounds.

**Optical activity due to the presence hetero atoms**

Chirality of organic compounds due to the presence of silicon, nitrogen, phosphorous, arsenic and sulphur atoms. Determination of R,S-configuration of these compounds using CIP rules.

**Transannular reactions**

Conformational analysis of medium rings.

Transannular reactions: Hydrolysis of medium ring epoxides and bromination of C<sub>8</sub>-C<sub>10</sub> cyclic dienes.

**UNIT-II**

**13h**

**Advanced Stereochemistry – II**

**Determining absolute and relative configuration**

- i). Chemical correlation of configuration: Methods without involving the chiral centre. Chemical transformation involving the chiral centre. Chemical correlation involving diastereomers.
- ii). Methods based on comparison of optical rotation: Distance rule, Rule of shift, Rule of optical superposition, Mill's rule, Method based on molecular rotation difference
- iii) The method of quasi-racemate.
- iv) Use optical rotatory dispersion curves:  $\alpha$ -axial haloketone rule and its applications, octant rule (application of these rules in the determination of absolute configuration of substituted cyclohexanones, decalones and cholestanones).
- v) Method based on anomalous X- ray scattering.

**UNIT-III**

**13h**

**Retrosynthetic analysis**

**Protecting groups**

Principle of protection of alcohols, amines, acids and carbonyl groups

**Disconnection approach**

Introduction to synthons, and synthetic equivalents, disconnection approach. Basic principles and terminologies used in disconnection approach. One group C-X and two group C-X disconnections. Chemoselectivity, reversal of polarity, cyclisation reactions.

**One group and C-C two group disconnections**: Synthesis of alcohols, carbonyl compounds and alkenes. Use of acetylides and aliphatic nitro compounds in organic synthesis. Diels-Alder

reaction, 1,3-difunctionalised compounds,  $\alpha,\beta$ -unsaturated compounds, carbonyl compounds condensations, 1,5- difunctionalised compounds. Michael addition and Robinson annelation.

#### **UNIT-IV**

13h

##### **Retrosynthetic analysis and synthetic route for some complex molecules**

Juvabione, aromadendrene, longifolene, cortisone, reserpine, vitamin-D, lycorane alkaloids and Prelog-Djerassi lactone.

#### **SUGGESTED BOOKS**

1. Stereochemistry, V R Dani, Asian books, New Delhi, 2015.
2. Principles of organic synthesis, R. Norman and J. M. Coxon, 3<sup>rd</sup> edition, CRC Press, 2015.
3. Organic synthesis: Concepts, methods and starting materials, 3<sup>rd</sup> edition, J-H. Furhlop and G. Li, Wiley-VCH, 2014.
4. Organic chemistry Volumes 1 and 2, 6<sup>th</sup> edition. I. L. Finar, Pearson – New Delhi, 2012.
5. Advanced organic chemistry, J. March, 4<sup>th</sup> Edn. John Wiley, 2008.
6. Stereochemistry D J Morris, RSC, Cambridge, 2001
7. Stereochemistry of organic compounds- Principle and applications, D. Nasipuri, 2<sup>nd</sup> edition, New Age International Publishers, 2001.
8. Stereochemistry, Nasipuri, D, New Age, 1999.
9. Advanced organic chemistry Part B, F. A. Carrey and J. Sundberg, Plenum Press, 1999.
10. Stereochemistry – conformation and mechanism, P S Kalsi, New Age International, Bangalore 1999.
11. Some modern methods of Organic Synthesis, W. Caruthers, Cambridge Uni. Press London, 2<sup>nd</sup> edition, 1998.
12. Organic synthesis, C. Willis and M. Wills, Oxford University Press, 1995.
13. Stereochemistry of carbon compounds, E. L. Eliel, S. H. Wilen and L. N. Mander, John Wiley & Sons, 1994.
14. Organic Chemistry, R. E. Ireland Prentice-Hall India, New Delhi, 1975.
15. Organic synthesis: The synthon approach, S. Warren, John Wiley & Sons, New York, 1<sup>st</sup>. edition.. 1983.
16. Designing organic synthesis: A disconnection approach, S. Warren, John Wiley & Sons, New York, 2<sup>nd</sup> edition, 1987.
17. Stereochemistry, Potapov, MIR, Moscow, 1984.
18. Stereochemisry, E L Eliel, TMH, New Delhi, 1984.

## C-402 OC: CHEMISTRY OF NATURAL PRODUCTS

52 Hours

### UNIT-I

13h

#### **Terpenoids**

Classification, nomenclature, occurrence and isolation. Isoprene rules. Stereochemistry of citral, farnesol, limonene, 1,8-cineole, menthols and borneols. Correlation of configurations of terpenoids.

Structure elucidation of camphene,  $\alpha$ -pinene,  $\beta$ -caryophyllene,  $\alpha$ -santonin and gibberillic acid. Synthesis and biosynthesis of the following:

Linalool,  $\alpha$ -terpineol, fenchone, eudesmol, abietic acid. Commercial synthesis of camphor.

Biosynthesis of squalene and cyclisation of squalene into  $\alpha$ -lanosterol and friedelene.

#### **Carotenoids**

Methods of isolation. Structural relationship of  $\alpha$ -,  $\beta$ - and  $\gamma$ -carotenes. Structure elucidation and synthesis of  $\beta$ -carotene.

### UNIT-II

13h

#### **Alkaloids**

Definition, nomenclature, occurrence, isolation, classification, General methods of structure elucidation. Synthesis and biosynthesis of the following alkaloids:

Ephedrine, hygrine, coniine and cocaine. Cinchona alkaloids: Cinchonine and quinine.

Opioid alkaloids: Morphine, codeine, thebiene and heroin.

Structure elucidation and synthesis of papaverine, reserpine and ergotamine. Photochemical synthesis of Nuciferine, coradyline and tylophorine.

### UNIT-III

13h

#### **Porphyrins**

Structure elucidation and synthesis of haemin, chlorophyll-a and vitamin-B<sub>12</sub> (synthesis of Vitamin-B<sub>12</sub> from cobyrinic acid).

#### **Nucleic acids**

Introduction, components of nucleic acids, nucleosides, nucleotides and oligonucleotides.

Structure elucidation and synthesis of nucleosides and nucleotides.

Chemical synthesis of oligonucleotides: Protecting groups for hydroxy group in sugar, amino group in the base and phosphate functions. Methods of formation of internucleotide bonds: DCC, phosphodiester approach, phosphotriester approach, phosphite triester and phosphoramidite methods. Solid phase synthesis of oligonucleotides.

### UNIT-IV

13h

#### **Prostaglandins**

Introduction, nomenclature, classification and biological role of prostaglandins. Structure elucidation and stereochemistry of PGE<sub>1</sub>, PGE<sub>2</sub> and PGE<sub>3</sub>. Synthesis of PGE<sub>1</sub> and PGE<sub>2</sub> by Corey's and Stork's approaches. Synthesis of PGE<sub>3</sub> by Upjohn's approach. Synthesis of

prostacyclin I<sub>2</sub> and thromboxane B<sub>2</sub>. Biosynthesis of prostaglandins.

### **Insect pheromones**

Introduction, classification. Pheromones in pest control. Syntheses of (one synthesis should be stereoselective synthesis)

- i) Grandisol (component of boll weevil pheromone)
- ii) Farenal (trail pheromone of pharaoh's ants)
- iii) Brevicommin (pheromone from *Dendroitis brevicomis*)
- iv) (+)- Disparlure (gypsy moth sex pheromone).
- v) 3,11-Dimethyl-2-nonacosanone (pheromone of German cockroaches).
- vi) Bombykol (sex pheromone of silkworm moth).
- vii) Multistriatin (Elm bark beetle sex pheromone).

### **SUGGESTED BOOKS**

1. Organic Chemistry Volume 2, 6<sup>th</sup> edition, I L Finar, Pearson – New Delhi, 2015.
2. Chemistry of natural products – a unified approach, 2<sup>nd</sup> edition, N R Krishnaswamy, Universities Press, Hyderabad, 2010.
3. Natural products: Their chemistry and biological significance, J. Mann, R. S. Davidson, J. B. Hobbs, D. V. Banthorpe & J. B. Harborne, Longman, UK, 1994.
4. Terpenes, J. Verghese, Tata McGraw-Hill, New Delhi, 1982.
5. Chemistry of terpenes and terpenoids, A. Newman, Academic Press, London, 1975.
6. Handbook of naturally occurring compounds Vol. II: Terpenes, T. K. Davon, A. I. Scott, Academic Press, NY, 1972.
7. Natural products chemistry Vol. I & II, K. Nakanishi, T. Goso, S. Ito, S. Natori & S. Nozoe, Academic Press, NY, 1974.
8. Total synthesis of natural products Vol. I & VI, Apsimon, John Wiley, NY, 1973-1981.
9. Chemistry of natural products Vol. I & II, O. P. Aggarwal, Goel Publishing House, 6<sup>th</sup> Edn. 1982.
10. Total synthesis of natural products: The chiral approach Vol. III, S. Hanessian Pergamon Press, 1983.
11. Total synthesis of steroids, Akhaun & Titov, Jerusalem, 1969.
12. Medicinal natural products: A biosynthetic approach, P. M. Dewick. John Wiley, Chichester, 1997.
13. The colours of life: An introduction to the chemistry of porphyrins and related compounds, L. R. Milgrom, Wiley Chichester, 1995.
14. Interpretation of the UV spectra of natural products, A.I. Scott, Pergamon Press, Oxford, 1964.
15. Spectral data of natural products Vol. I- K. Yamaguchi, Elsevier Publishing Co, London, 1970.
16. Chemistry of natural products: A unified approach, N. R. Krishnaswamy, University Press, India, 1999.

## C-403 OC: INDUSTRIAL ORGANIC CHEMISTRY

52 Hours

### UNIT-I

13h

#### **Dyes**

Introduction. Modern theories of colour and chemical constitution. Methods of applying dyes to fabrics. A general study of the following: Mordant dyes, vat dyes, disperse dyes, fibre reactive dyes, sulphur dyes, cyanine dyes, solvent dyes and pigment dyes with examples. Direct azo dyes (congo red), acid azo dyes, (Ponceau2R, Naphthol blue black 6B), basic azo dyes (Chrysoidin G, Bismarck brown), developed dyes (indigo).

Fluorescent brightening agents (Tinopal).

Cyanine dyes: Quinoline blue and sensitol red. Chemistry of colour developers, and instant colour processes.

Synthesis and applications of malachite green, rhodamine-B, phenolphthalein and methyl orange. Triphenylmethane dyes: crystal violet, *p*-rosaniline, acid chrome Violet-K.

Application of dyes in photography, visual displays, biological studies and electronics.

### UNIT-II

13h

#### **Heterocyclic Chemistry**

*Small ring heterocycles:* Properties and reactions of 3- and 4- membered heterocycles: oxiranes, thiranes, aziridines, azetidines, oxetanes and thietanes.

*Benzo-fused heterocycles:* Synthesis and reactions of benzofurans, benzothiophenes, benzoxazoles, benzothiazoles and benzimidazoles.

*Six-membered heterocycles with two or more heteroatoms:* Synthesis of Diazines, triazines, tetrazines and thiazines.

*Seven and large membered heterocycles:* Synthesis and reactions of azepanes, oxepines, thiepinines, diazepines, thiazepines, azocines, diazocines, dioxocines and dithiocines.

*Heterocycles containing P, As, Sb and Bi:* Synthesis of 5- and 6- membered heterocycles with P, As, Sb and Bi.

*Mesoionic compounds:* General classification, chemistry of some important meso-ionic heterocycles of type-A and type-B and their applications.

### UNIT-III

13h

#### **Organometallic Chemistry**

*Organosilicons:* Preparation and reactions of trialkylsilyl halides with ethers, epoxides, esters, carbamates and acetals. Peterson olefination.

*Organotins:* Preparation and reactions of tri-*n*-butyltin hydride, Barton decarboxylation and Barton- McCombie reaction.

*Organomercurials:* Preparation, electrophilic substitution reactions, Solvomercuration-demercuration reaction. Cyclopropanation of alkenes.

*Organozincs:* Preparation, reaction with compounds containing acidic protons, reaction with C-C multiple bonds, trans-metallation, addition reactions of zinc reagents with carbonyl compounds. Simmons Smith and Reformatsky reaction.

*Organolithiums:* Preparation, deprotonation reaction, nucleophilic addition reactions, reactions with imines, nitriles and isonitriles.

*Organocopper reagents:* (Gilman reagents-lithium dialkyl cuprates): Preparation, reactions with alkyl, allyl, vinyl, benzyl and aryl halides, aldehydes, ketones (including  $\alpha,\beta$  - unsaturated carbonyl compounds) and epoxides.

*Organoseleniums:* Preparation, synthesis of alkenes from alkyl halides and  $\alpha,\beta$  - unsaturated carbonyl compounds from carbonyl compounds.

*Organoaluminiums:* Preparation, hydroalumination and carboalumination of alkenes, nucleophilic addition reactions with carbonyl compounds and Hydrocyanation. Preparation of alkenyldialkylalanes and their reactions.

## UNIT-IV

13h

### **Polymers**

Preparation, properties, classification (natural and synthetic), nomenclature and importance of polymers. Properties of polymers (molecular weight, glass transition temperature – T<sub>g</sub>, solubility, viscoelasticity etc). Basic concepts and techniques in polymer chemistry. Monomers, repeat units, degree of polymerization. Homo-, co-, ter-, addition and condensation polymers with examples. General structures of polymers. Tacticity. Techniques of polymerization (bulk, emulsion, co-polymerization). Stereochemistry – configuration. Thermoplastics, thermosets and elastomers. Polymer processing techniques, additives for improvement of polymer properties, spinning of industrial polymers, wet and dry. Melt spinning. Application of polymers in fibres, composites, adhesives etc. Polymer degradation – thermal and oxidative-reductive processes.

Natural polymers: Polyisoprenes, and chitosan. Synthesis and applications of vinyl polymers: (polyethylene, poly styrene, polypropylene, PVC, chlorinated PVC, teflon and polymethacrylate). Polyesters: (Polyethylene terephthalate). Polyamides: Kevlar and Nomex, Bakelite. Polyureas, polyurethanes, polyimides and polysulfones.

### **SUGGESTED BOOKS**

1. Modern methods of organic synthesis, W. Carruthers and I Coldham, 4<sup>th</sup> edition, Cambridge Univ. Press, Cambridge, 2014.
2. Advanced organic chemistry – organic synthesis heterocycles and biomolecules, N Tewari, Books and Allied Publishers, Kolkata – 2013.
3. Heterocyclic Chemistry, J. A. Joule, K. Mills and G. F. Smith, 5<sup>th</sup> edition, Blackwell, Chichester, 2010.
4. Synthetic Dyes, G R Chatwal, Himalaya, New Delhi – 2009.
5. Advanced Organic Chemistry, J. March, 4th edition, John Wiley, 2008.
6. Technology of synthetic dyes, pigments and intermediates, EIRI, New Delhi – 2005.
7. Polymer science, V R Gowariker, N V Vishwanathan, J Sreedhar, New Age International, New Delhi – 2005.
8. Industrial organic chemistry, 4<sup>th</sup> edition, K. Weissermel, H,-J Arpe, translated by C R Lindley, S Hawkins, Wiley-VCH, Weinheim, 2003.
9. Handbook of heterocyclic chemistry, 2<sup>nd</sup> edition, A R Katritzky, Pergamon, Oxford, 2000.
10. The chemistry of colour application R M Christie, R R Mather and R H Wardman, Blackwell, Oxford, 2000.
11. Stereochemistry of Organic Compounds, D Nasipuri, New-Age International, 1999.
12. Heterocyclic Chemistry, Vols. 1-3, R. R. Gupta, M. Kumar and V. Gupta, Springer Verlag, 1998.
13. Comprehensive Heterocyclic Chemistry, A. R. Katritzky and C. W. Rees, Eds. Pergamon Press, 1996.
14. The Chemistry of Heterocycles, T. Eicher and S Hauptmann, Thieme, 1995.

15. Introduction to synthetic polymers, I M Campbell, Oxford, 1994
16. Heterocyclic Chemistry, T. L. Gilchrist, Longman, 1992.
17. Textbook of polymer science, 3<sup>rd</sup> edition, F W Billmeyer, Wiley, 1984.
18. Contemporary Heterocyclic Chemistry, G. R. Newkome, and W. W. Paudler, Wiley-Inter Science, 1982.
19. An introduction to Heterocyclic Compounds, 3<sup>rd</sup> edition, R. M. Acheson, John Wiley, 1976.
20. The chemistry of synthetic dyes, K Venkataraman Ed., Vols 1-7, Wiley, New York, 1971.
21. Synthetic dyes in biology, medicine and chemistry, E Gurr, Academic, NY, 1971.

## C-404 OC: MEDICINAL ORGANIC CHEMISTRY

52 Hours

### UNIT-I

13h

#### **Basic Concepts of Medicinal Chemistry**

Basic terms defined: Drug, medicine, pharmacy, pharmaceuticals, toxicology, pharmacodynamics agents, pharmacophore, pharmacodynamics, metabolites and anti-metabolites, chemotherapy. LD<sub>50</sub>, ED<sub>50</sub>, IC<sub>50</sub> and ID<sub>50</sub>.

Classification of drugs on the basis of therapeutic action. Drug Discovery. Identification of Lead. Lead Modification. SAR. Identification of pharmacophore. Structure-activity relationship structure modification to increase potency and the therapeutic index by homologation; chain branching; ring-chain transformation. Bioisosterism. Concept of prodrugs and soft drugs. Properties of soft drugs.

Basics of drug receptor interactions. Theories of drug activity. Hansch equation. QSAR. Computer-aided drug design and molecular modeling.

### UNIT-II

13h

#### **Steroids**

Occurrence. Nomenclature, basic skeleton, Diels hydrocarbon and stereochemistry. Isolation, structure and structural elucidation of sterols and bile acids (determination of ring size, nature of side chain, position of angular methyl and stereochemistry of ring junctions). Sex hormones and corticosteroids. Synthesis of cholesterol, estrone, progesterone, androsterone, testosterone. Photo products of ergosterol- vitamins D. Barton reaction for the synthesis of aldosterone.

Marker degradation. Brief discussion of homosteroids, norsteroids and oral contraceptives. Synthesis of (*dl*)-norgestrel and ethinyl oestradiol.

### UNIT-III

13 h

#### **Synthesis and mechanism of drug action and of the following classes of drugs**

Introduction and general mode of action of:

*Antibiotics*: Discovery/synthesis of penicillins, cephalosporin-C, streptomycin, chloromycetin and tetracyclins (terramycin and aureomycin).

*Antipyretics, analgesics and non steroidal anti-inflammatory drugs*: Aspirin, paracetamol, phenacetin, novalgin, phenylbutazone and ibuprofen.

*Antidiabetics*: Sequence of A- & B- chains of insulin, glibenclamide, metformin, ciglitazone.

*Antihistamines*: Methapyrilene, chlorpheniramine.

*Antivirals*: Acyclovir, amantidine, rimantidine and zidovudine.

*Antineoplastic agents*: alkylating agents and antimetabolites in treatment of cancer. Synthesis of mechlorethamine, cyclophosphamide, melaphan, uracil mustard and 6- mercaptopurine.

*Cardiovascular drugs*: Synthesis of amyl nitrite, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol, oxyprenol.

## UNIT-IV

13h

### **Local anti-infective agents**

Introduction synthesis and general mode of action. Sulfa drugs: sulphanilamide, dapsone.

Antiparasitic chemotherapy: furazolidone, nalidixic acid, ciprofloxacin, chloroquin and primaquin, DOTS treatment using p-aminosalicylic acid, isoniazide, ethionamide, ethambutal.

Antifungals: griseofulvin, fluconazole, econazole.

Psychoactive drugs- chemotherapy of the mind: Synthesis of utility of the following: pethidine, methadone, benzodiazepines: diazepam, oxazepam, chlorazepam, alprazolam, chlorpromazine, butyrophenones, buspirone, barbiturates: phenobarbital, phenytoin, ethosuximide, trimethadione, , thiopental sodium, glutethimide. SAR with opioid alkaloids.

### **SUGGESTED BOOKS**

1. An Introduction to Medicinal Chemistry, 6<sup>th</sup> edition, P Graham, Oxford, 2017.
2. The Organic Chemistry of Drug Design and Drug Action, R B Silverman, and M W Holladay, 3<sup>rd</sup> edition, Academic Press, Amsterdam, 2014.
3. Organic chemistry Vol.II, I. L. Finar, 6<sup>th</sup> Edn. Pearson – New Delhi, 2012.
4. Foye's Principles of Medicinal Chemistry, 6th Edn., T L Lemke and D A Williams Eds., Lippincott, Williams and Wilkins, 2008
5. Medicinal Chemistry, T Nogrady and D F Weaver, 3<sup>rd</sup> edition, Oxford, 2006
6. Goodman and Gilman's Pharmacological Basis of Therapeutics, 11th Edn., Tata McGraw-Hill, 2005.
7. Burger's Medicinal Chemistry and Drug Discovery, Vols. 1-6 Ed. D.J. Abraham, John Wiley, 2003
8. 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.
9. Medicinal Chemistry – G R Chatwal, Himalaya, New Delhi, 2002.
10. Instant Notes Medicinal Chemistry, P Graham, Viva, New Delhi, 2002
11. Medicinal Chemistry, A Kar, Wiley, 2000.
12. An Introduction to Drug Design, S.S. Pandeya and J.R. Dimmock, New Age International, 1999.
13. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley, 1998.
14. Medicinal natural products: A biosynthetic approach, P. M. Dewick. John Wiley, Chichester, 1997.
15. Synthetic drugs, G. R. Chatwal, Himalaya, New Delhi, 1995.
16. Natural Products Chemistry Vol 1 and 2, G R Chatwal, Himalaya, New Delhi, 1990
17. Comprehensive Organic Chemistry, Vol. 5 (Antibiotics), D. H. R. Barton, W. D. Ollis, Pergamon Press, NY, 1979.
18. Total synthesis of natural products: The chiral approach Vol.III, S. Hanessian Pergamon Press, 1983.
19. Total synthesis of steroids, Akhaun & Titov, Jerusalem, 1969.
20. Natural products: Their chemistry and biological significance-J. Mann, R S Davidson, J. B. Hobbs, D. V. Banthorpe & J. B. Harborne, Longman, UK, 1994.
21. Natural products chemistry Vol. I & II, K. Nakanishi, T. Goso, S. Ito, R. Natori & S. Nozoe, Academic Press, NY, 1974.
22. Chemistry of natural products Vol. I & II, O. P. Aggarwal, Krishna Prakashan,

2015.

23. Total synthesis of natural products: The chiron approach, S Hanessian Pergamon Press, 1983.

**PRACTICALS**  
(4 days a week, 4 hours a day)

**C-405 OC: PREPARATION OF INDUSTRIAL IMPORTANCE**

1. Preparation of NBS from succinic acid and its application in allylic/benzylic brominations
2. Photochemical preparation of benzpinacolone from benzophenone.
3. Preparation of tetracyclone. Generation of benzyne and its trapping with tetracyclone.
4. Synthesis of 2-phenylindole from phenylhydrazine
5. Oxidation of anthracene to anthraquinone and conversion to anthrone.
6. Reduction of benzoin to stilbene.
7. Esterification of 4-nitrobenzoic acid and conversion to benzocaine.
8. Preparation of tetraphenyldihydrophthalic anhydride from N-phenylglycine.
9. Preparation of 2,4,5-triphenyloxazole from benzoin.
10. Biosynthesis of ethanol from sucrose.
11. Preparation of methyl red/methyl orange from aniline.
12. Synthesis of benzimidazole from urea.
13. Conversion of 2-naphthol to 1-bromo-2-naphthol.
14. Synthesis of hippuric acid.
15. Synthesis of 1,2,3,4-Tetrahydrocarbazole.
16. Diels-Alder cycloaddition of anthracene with maleic anhydride.
17. Synthesis of 2,3-diphenylquinoxaline.
18. Green synthesis of acetanilide from aniline.
19. Photo-dimerisation of *trans*-cinnamic acid to  $\beta$ -truxinic acid.
20. Preparation of caprolactam from cyclohexanone. Conversion to Nylon-6.
21. Synthesis of Nylon-6,6.
22. Synthesis of tetraphenylporphyrin.
23. Preparation of indigo from anthranilic acid.
24. Synthesis of fluorescein and eosin from resorcinol.
25. Preparation of urea-formaldehyde resin (bakelite).

**C-406 OC: EXTRACTIONS & SEPERATIONS**

1. Extraction of piperine from pepper.
2. Extraction of caffeine from tea leaves.
3. Extraction of hesperidine from citrus fruits rinds'.
4. Extraction of azelaic acid from castor oil.
5. Extraction of DNA from onion peels.
6. Extraction of lycopene from tomatoes.
7. Isolation of essential oils from cumin.
8. Isolation of essential oils from rose petals.
9. Isolation of curcuminoids from turmeric powder.
10. Isolation and separation of lactose and casein from milk.
11. Isolation and separation of pigments chlorophyll and  $\beta$ -carotene from spinach.

12. Separation of caffeine from tannins by sublimation.
13. Natural product isolation using steam distillation and liquid phase extraction of thymol, camphor, and citral, monoterpenes sharing a unified biosynthetic precursor
14. Isolation of enzymes: Lipase and Sucrase.
15. Extraction of groundnut/coconut/eucalyptus oils
16. Separation of p-rosaniline and methyl red by column chromatography.
17. Separation of amino acids by paper chromatography.
18. Separation of carbohydrates by thin layer chromatography.
19. Separation of *o*- and *p*-nitroanilines by thin layer chromatography.
20. Separation of anthracene from anthracene picrate.
21. TLC of analgesic drugs: acetaminophen, aspirin, caffeine, ibuprofen and salicylamide.

### C-407 OC: INSTRUMENTAL METHODS AND QUANTITATIVE ANALYSIS

#### Instrumental methods in organic analysis

1. Recording/predicting/downloading s the UV, IR, NMR and GC-MS spectra from web sites of the compounds prepared in third semester.
2. Structural elucidation of organic compounds with the help of spectra provided by the instructors/examiners.

#### Quantitative analysis

##### Estimations:

1. Estimation of Nitro group by reduction using  $\text{SnCl}_2$ .
2. Estimation of Nitrogen by Kjeldahl's method.
3. Estimation of an acid in presence of an amide.
4. Estimation of an ester in the presence of an acid.

### C-408 OC: QUALITATIVE ANALYSIS OF BINARY MIXTURES

Separation of binary mixture of organic compounds by organic solvents/aqueous techniques. Identification of the separated component/s by systematic qualitative organic analysis.

#### SUGGESTED BOOKS

1. Organic Synthesis Collective Volumes 1 to 11, 1956-2019. (Freely available on the web)
2. Advanced practical organic chemistry, 3<sup>rd</sup> edition, J Leonard, B Lygo and G Proctor, Routledge, CRC Press, London, 2013.
3. Practical Organic Chemistry, 5<sup>th</sup> edition, Furniss B S, Hannaford, A J, Smith, P W G and Tatchell, A R, Pearson, New Delhi – 2012.
4. Practical organic chemistry F.G. Mann and B. C. Saunders, Pearson, 2009.
5. Laboratory Techniques in Organic Chemistry, V K Ahluwalia, Pooja Bhagat and Renu Aggarwal, I K International Publishing House, New Delhi, 2005.
6. Intermediates for Organic Synthesis, V K Ahluwalia, Pooja Bhagat, Ramesh Chandra and Renu Aggarwal, I K International Publishing House, New Delhi, 2005.
7. Text book of practical organic chemistry, A. I. Vogel, Pearson, 5<sup>th</sup> Edition, Delhi, 2004.
8. The systematic identification of organic compounds, 8<sup>th</sup> edition, R L Shriner, C K F Hermann, T C Morrill, D Y Curtin and R C Fuson, Wiley, 2004
9. Organic structures from spectra, 3<sup>rd</sup> edition, L D Field, S Sternhall, J R Kalman, Wiley, Sydney, 2002.
10. Laboratory Experiments for Organic and Biochemistry, IV edition, F. A. Bettelheim and J. M

Landesberg, Harcourt College Publishers, Orlando. FL, 2001

11. Structural analysis of organic compounds by combined application of spectroscopic studies, J T Clerc, E Pretsch, J Seibl, Elsevier, Amsterdam, 2001.
12. Comprehensive practical organic chemistry: Preparation and quantitative Analysis, V. K. Ahluwalia, R. Aggarwal, Universities Press (India), 2000.
13. Comprehensive practical organic chemistry: Qualitative analysis, V. K. Ahluwalia, S. Dhingra, Universities Press (India), 2000.
14. Natural products, Laboratory manual, Ikan, 2000.
15. An advanced course in practical chemistry, A. Ghoshal, B. Mahapatra and A. K. Nad, New central book agency, Calcutta, 2000.
16. Interpreting organic spectra, D Whitaker, RSC, Cambridge, 2000.
17. Organic experiments, L. F. Fieser, 2<sup>nd</sup> Edn. D. C. Heath & Co. USA, 1974-2000.
18. Organic Laboratory Chemistry – Microscale, II edition, B. H Inshaw, R Wooley Outernet Publishing, Eden Prairie, MN, 1999.
19. A laboratory manual of qualitative organic analysis, H.T. Openshaw, Univ. Press, 1999.
20. Introduction to Organic Laboratory Techniques – a microscale approach, II edition, D L Pavia, G M Lampman, G S Kriz and R G Engle, Saunders College/Harcourt Publishing, 1999.
21. Techniques and experiments for advanced organic laboratory, C. M. Garner, John Wiley, NY, 1997.
22. Advanced practical organic chemistry, J. Mohan, Vol. I and II, Himalaya Publishing House, 1992.
23. Practical organic chemistry (Quantitative analysis), B. B. Dey, M V Sitaraman and T. R. Govindachari, Allied Publishers, New Delhi, 1992.
24. Detection and identification of organic compounds, M Vecera and J Gasparic, Springer, 1972.
25. Semi-micro qualitative organic analysis, 3<sup>rd</sup> edition, N D Cheronis, J B Entrikin and E M Hodnett, Wiley, New York, 1967.

**THIRD SEMESTER**  
**PHYSICAL CHEMISTRY SPECIALISATION**  
**Ch-301 PC: APPLIED ELECTROCHEMISTRY**

**52 Hours**

**UNIT-I**

**Electroanalytical methods**

**13h**

*Voltametry:* Definition, concentration polarization, ideal and non-ideal polarized electrodes, Faradaic and non-faradaic currents.

*Polarography:* Construction of dropping mercury electrode (DME), advantages and limitations. Principle of normal dc polarography, half-wave potential, qualitative analysis using polarograms. Types of currents obtained at a DME. Ilkovic equation, factors affecting diffusion controlled current, quantitative analysis based on Ilkovic equation. current-potential relation for a cathodic wave, anodic wave and composite wave, test for the reversibility of a process at DME, factors that set the sensitivity and selectivity limits in normal dc polarography.

*Advanced polarographic techniques:* Fast polarography, normal pulse polarography, differential pulse polarography, ac polarography.

*Stripping voltametry:* Hanging drop mercury electrode (HDME), principles and applications of cathodic and anodic stripping voltametry.

*Cyclic voltammetry:* Principle, experimental setup, quantitative analysis. Diagnostic criteria for reversible, quasi-reversible and irreversible processes. Study of coupled chemical reactions like  $E_rC_r$ ,  $C_rE_r$  and  $E_rC_iE_r$ .

*Chrono methods:* Basic concepts, methodology and applications of chronoamperometry, chronopotentiometry and chronocoulometry.

*Hydrodynamic electrodes:* Construction and use of rotating disc and rotating ring disc electrodes in the electrochemical studies

*Membrane electrodes:* Ion-selective membrane electrodes-construction and applications of solid state and liquid membrane electrodes, ion selective field effect transistor and Molecular(gas) sensing probes. Problem solving.

**UNIT II**

**13h**

**Electrochemical Energy conversion and storage**

*Batteries:* History and basics, classification, characteristics with units-voltage, current, capacity, electricity storage density, energy density, power density, energy efficiency, cycle life, shelf life.

*Primary batteries:* Construction, reactions and uses of Leclanche' dry cell, alkaline Leclanche cell, zinc-silver oxide cell.

*Secondary batteries:* Construction, working (charge-discharge reactions), applications advantages and of Pb-acid and Ni-Cd batteries.

*Hybrid Batteries: Metal-air batteries-* meaning, Zn-air battery, Fe-air battery, Charging of metal-air battery, Metaloxide-hydrogen/hydride batteries, advantages and limitations of these cells

*Lithium batteries:* Primary and secondary lithium battery, Li-ion battery and Lithium ion-polymer battery.

*Electrochemical supercapacitors:* comparative meaning of capacitor, electrolytic (super) capacitor and ultracapacitors, materials for construction, applications, advantages and limitations.

*Fuel cells:* Energy efficiency of electrochemical and thermal conversion (Carnot limitation). Definition of fuel cell, classification. Fuel cell efficiency- thermodynamic, electrochemical, practical efficiency. Electrode (anode and cathode) mechanism of fuel cell, Brief description on construction, working principle and applications of each type fuel cells. An account of electrocatalysts, proton exchange membrane (PEM) fuel cells and direct methanol fuel cell. Problems solving.

### UNIT-III

#### **Surface Modification techniques(Metal finishing)**

**13h**

Definition Important processes of metal finishing, technological importance of metal finishing.

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

*Metallic coating:* Preparation of substrate surface, electroplating of Cu and Cr. Applications of Au and Ag platings.

*Solar selective coatings:* Characteristics, methods of preparation and applications.

*Techniques of electroplating:* Galvanizing, Anodizing, Phosphating, Chromating.

Electroless plating: Definition, advantages over electroplating, pretreatment of substrates, an account of electroless plating of Ni including applications.

*Testing of coats:* Principles of measurement of coating thickness, adhesion, porosity, corrosion resistance, reflectance, and hardness. A brief account of surface analysis by XPS and AES techniques.

*Industrial effluent treatment:* An account of removal of toxicants like, CN, Cr, Pb and Cd from plating industrial effluent. Problems solving

#### **Electrochemical synthesis**

Special features of electrochemical synthesis compared to conventional synthesis-reaction variables (electrode material, electrode potential, solvent, supporting electrolyte, temperature, agitation) in electrochemical synthesis. Two examples for electroorganic, electroinorganic and electrochemical nanoparticles synthesis with mechanism.

### UNIT-IV

#### **Corrosion and its Prevention**

**13h**

Introduction, dry and wet corrosion, theories and mechanisms of wet (electrochemical) corrosion, thermodynamic aspects of corrosion, kinetic aspects- determination of rates of corrosion by linear polarization, Tafel extrapolation and impedance techniques. Factors influencing the rate of corrosion- metal and environmental.

Methods of corrosion prevention: Cathodic protection, anodic protection, use of corrosion inhibitors, use of organic coatings.

Passivity: Definition, current potential diagram, characteristics of passivity, theory and mechanism of passivation, flade potential, trans passivity. Use of ellipsometric technique in the study of passivating films. Problems solving

### **Bioelectrochemistry**

The electrochemical interface between biomolecules, cellular membrane, transmembrane potential, bilayer lipid membranes, electroporation, biological electron transport, electrochemistry of redox enzymes, biological membrane and membrane mimics. Biosensors- NADP, glucose, phenolic. Bioelectroanalysis: Electrolysis and Electrodialysis.

### **SUGGESTED BOOKS**

1. Modern Electrochemistry, Vol.1,2A and 2B by Bockris and Reddy, Plenum,N.Y (2000).
2. Polarography and Allied Techniques by V SuryanarayanaRao, UniversitiesPress (India) Pvt. Ltd., Hyderabad(2002).
3. Basic concepts of Analytical Chemistryby S M Khopkar, New Age International Publishers, third edition, New Delhi,2008.
4. Electrochemical Methods- Fundamentals and Applications, 2<sup>nd</sup>Edn, by A J Bard and L R Faulkner, John Wiley & Sons Inc., New York(2001).
5. Chemical and Electrochemical Energy systems by Narayan andViswanathan, Hyderabad, Universities Press (india) Pvt. Ltd., Hyderabad(2002).
6. Understanding Batteries, RM Dell and DAJ Rand, 2001.6. Fuel cells and their applications, Karl kordesh, gunter,Simader, VCH-Weinheim,Cambridge,1996.
7. Fundamentals of electrochemical deposition, Milan Paunovic and Mordechay Schlesinger, Wiley- interscience publications, New York,1998
8. Electrodeposition and Corrosion Control, J. M. West, J. Wiley W. Revie (ed.): Corrosion Handbook, Electrochemical Society Series, John Wiley and Sons(2000).
9. Electrochemistry and corrosion science, Nestor Perez, Springer (India) pvt. Ltd.,2004
10. Principles and Prevention of Corrosion, D. A. Jones, Macmillan Publ. Co.(1996).
11. Bioelectrochemistry: Fundamentals, experimental techniques and application, P. N. Bartlett, Wiley& Sons(2008).
12. Synthetic organic Electrochemistry by A M Fry, 2<sup>nd</sup>Edn, Wiley 1989.

## Ch-302 PC: QUANTUM CHEMISTRY & SURFACE CHEMISTRY

### UNIT-I

52 Hours

#### **Quantum Chemistry-I: Theories of valence**

13h

Introductory aspects: Linear and non-linear variation functions. Secular equations. Coulombic, exchange, normalization and overlap integrals. Secular determinants. Molecular orbital (MO) theory, LCAO-MO approximation, application to Hydrogen molecule ion ( $H_2^+$ ), energy levels of  $H_2^+$ , bonding and antibonding molecular orbitals, electron distribution, potential energy diagrams, comparison of theoretical and experimental values of energy. Valence bond (VB) theory of  $H_2$  molecule, the Heitler-London method, energy levels, energy distribution. Various modifications of the Heitler-London wavefunction.

Comparison of MO and VB theories. Ionic terms, fractional ionic characters and its importance, Equivalence of simple MO and VB methods ion-covalent resonance and configuration interaction. LCAO treatment of diatomic molecules, LCAO forms of simple wave function and molecular orbitals. Notations of molecular orbitals: full notation, Mulliken notation. MO configuration of homo- and hetero-nuclear diatomic molecules. Molecular electric terms. Bond order, stability and magnetic behavior of molecules from M.O. diagrams, isoelectronic systems. Correlation diagrams, non-crossing rule.

### UNIT-II

#### **Quantum Chemistry-II**

13h

The HF-SCF-LCAO method. Directed valence, hybridization, Expressions for hybrid orbitals in terms of wave functions of s and p orbitals and explanation of directed valences of  $sp$ ,  $sp^2$ , and  $sp^3$  hybrid orbitals. Hybridization involving d-orbitals, Localized and non-localized molecular orbitals in polyatomic molecules ( $H_2O$ ).

Huckel molecular orbital theory: Outline of the method including assumptions. Application to ethylene, allyl radical, cyclopropenyl radical, butadiene, cyclobutadiene, bicyclobutadiene and benzene. Calculation of delocalization energy, charge density,  $\pi$ -mobile bond order and free valence.

### UNIT-III

#### **Surface Chemistry-I**

13h

Review of adsorption curves, Adsorption-desorption, Adsorption forces, Heat of adsorption- Types, Measurements of heat of adsorption (Calorimetric and Clausius Clapeyron method), Measurement of adsorption isotherms, (Volumetric and Gravimetric methods), Determination of entropy of adsorption, Electrostatic adsorption, adsorption indicators and their applications. Volcanic curves. Applications of adsorption.

Adsorption kinetics: Kinetics of chemisorption (Hertz-Knudsen equation), Chemisorptive bond, Competitive adsorption, Mechanism of some catalyzed surface reactions, Kinetic effects of surface heterogeneity, Kinetic effects of interactions, Potential energy curves for adsorption, Transition state theory of surface reactions, Rates of desorption, Kinetics of bimolecular surface reactions, Langmuir-Hinshelwood Mechanism, Langmuir-Rideal mechanism, Rideal-Eley mechanism and their comparison.

#### **UNIT-IV**

##### **Surface Chemistry-II**

**13h**

Adsorption theories: Polanyi's potential theory and Polarization theory. Hysteresis of adsorption. Surface structure: Surface mobility, Surface heterogeneity, Surface area and its determination by point-B method, Harkins-Jura method, Radioactive tracer method and Benton and White method. Importance of surface area.

Examination of surfaces by Interferometer method, Scanning electron microscopy (SEM), Low energy electron diffraction method (LEED method), Field Emission spectroscopy, Auger electron spectroscopy (AES), STM, and TEM.

#### **SUGGESTED BOOKS**

1. Molecular Quantum mechanics, P.W. Atkins and R.S. Friedman, Oxford university press (1997).
2. Introductory Quantum Chemistry by A. K. Chandra, Tata McGraw Hill (1994).
3. Quantum Chemistry by R.K. Prasad, 3<sup>rd</sup> Edn, New Age International (2006).
4. Quantum Chemistry by Ira N. Levine, Prentice Hall, New Jersey (1991).
5. Quantum Chemistry by Donald A McQuarrie, Viva Books Pvt. Ltd. New Delhi, India, Published in arrangement with University Science books, Sausalito, CA, USA (2003).
6. Physical chemistry of surfaces by A. W. Adamson, Interscience Publishers Inc., New York (1967).
7. Surface Chemistry: Theory and Applications by J.J Bikertman, Academic Press, New York (1972).
8. Chemical Kinetics by K.J Laidler, 3<sup>rd</sup> Edn. Harper International Edn., (1987).
9. Text Book of Physical Chemistry by S. Glasstone, MacMillan India Ltd. 2<sup>nd</sup> Edn., (1986).
10. Physical chemistry, R J Silbey, R A Alberty and M G Bawendi Edn, Wiley (2009).
11. Physics at surfaces, A Zangwill, Cambridge University Press (1988).
12. Surface crystallography, L J Clarke, Wiley-Interscience (1985).

**Ch-303 IC/OC/PC: ORGANIC SPECTROSCOPY**  
**(Common to inorganic/ organic/ physical chemistry)**

52 Hours

**UNIT-I**

13h

**Ultraviolet/ visible spectroscopy**

Instrumentation. Classification of electronic transitions. Substituent and solvent effects.

UV spectral study of alkenes, polyenes,  $\alpha,\beta$ -unsaturated carbonyl and aromatic compounds. Empirical rules for calculating  $\lambda_{\max}$ .

**Vibrational Spectroscopy: Infrared and Raman spectroscopy**

Instrumentation. Sampling techniques, Group frequencies, factors affecting group frequencies, Bond order, Mass effect, Conjugation, Inductive, resonance, steric effects. Intramolecular interactions. Application of IR in the study of H-bonding, stereoisomerism and tautomerism. Complementarity of IR and Raman. Identification of the following organic compounds by IR: alkanes, alkenes, alkynes, aromatic compounds, aldehydes, ketones, alcohols, acids, acid chlorides, amides, amines, esters, halides and nitro compounds etc. Problems using UV and IR.

**UNIT-II**

13h

**Nuclear magnetic resonance spectroscopy-I**

Introduction, Magnetic properties of nuclei- Resonance condition. Nuclear spin, population of nuclear spin levels and NMR isotopes, Relaxation methods. Instrumentation and sample handling, FT-NMR.

Chemical shift. Mechanism of shielding and deshielding in Alkanes, Alkyl halides, Alkenes, Aromatic compounds, Carbonyl compounds and Annulenes. Pascal's triangle-low and high resolution, spectrum of ethanol. Karplus Curve, Diamagnetic and paramagnetic effects and magnetic anisotropy. Equivalence of protons-chemical and magnetic equivalence. Spin-systems: First order and second order coupling of AB systems, Simplifications of complex spectra.

Problems.

Spin-spin interactions: AX, AX<sub>2</sub>, AX<sub>3</sub>, AMX, AB types. Vicinal, geminal and long range coupling-Spin decoupling. Chemical shift reagents and deuterium exchange. Stereochemistry and hindered rotations. Temperature effects.

**UNIT-III**

13h

**Nuclear magnetic resonance spectroscopy-II**

CIDNP, Nuclear Overhauser effect (NOE). Factors influencing coupling constants and Relative intensities. Protons attached to elements other than carbon.

<sup>13</sup>C NMR Spectroscopy: Range and factors affecting chemical shifts of alkanes, alkyl halides, alkenes, alcohols, ethers, alkynes, carbonyl compounds and aromatics..

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

Explanation of the principle, applications to structure elucidation and stereochemistry of simple organic molecules.

Dynamic NMR.

NMR spectroscopy of other nuclei with spin I = ½. Introduction to <sup>15</sup>N, <sup>19</sup>F, <sup>29</sup>Si and <sup>31</sup>P NMR spectroscopies.

**Mass spectrometry and Composite Problems:**

Basic principles-instrumentation – ion production-ion analysis-magnetic sector instruments  
Quadrupole mass spectrometers. Time of flight mass spectrometers-ion cyclotron resonance  
spectrometers- Mass spectrum-molecular ion-types of ions in mass spectra and effects of  
isotopes on mass spectra. Methods of ionization, EI, FAB MALDI and ESI methods.  
Fragmentation of alkanes, alkenes, aromatics, alkyl halides, alcohols, aldehydes, ketones,  
acids, esters, ethers, amines, nitro and halo compounds peptides, Nitrogen rule, Factors affecting  
cleavage patterns. McLafferty rearrangement. Determination of molecular formula. Problems.

Use of HRMS to determine exact molecular formulae of compounds.

Application of UV, IR, NMR and MS methods and chemical reactions in the structure  
elucidation of organic compounds – composite problems.

**SUGGESTED BOOKS**

1. Spectroscopic methods in organic chemistry, 7<sup>th</sup> edition, D Williams and I Fleming, Springer International Publishing, Berlin – 2019
2. Fundamentals of molecular spectroscopy 5<sup>th</sup> edition, C N Banwell, E M McCash, H K Choudhury, Tata McGraw Hill, New Delhi - 2015
3. Spectrometric identification of organic compounds, R. M. Silverstein, F X Webster, D J Kiemle and D L Bryce, 8<sup>th</sup> Wiley student edition, New Delhi, 2015.
4. Organic spectroscopy, W. Kemp, Macmillan, London, 2011.
5. Introduction to spectroscopy, 4<sup>th</sup> edition, D. L. Pavia, G. M. Laupman and G. S. Kriz, Harcourt College Publishers, 2009.
6. Structure determination of organic compounds E Pretsch, P Buhlmann and M Badertscher, Springer-Verlag, Berlin – 2009.
7. Spectroscopic methods in organic chemistry, M Hesse, H Meier, B Zeeh, 2<sup>nd</sup> edition, Thieme, Stuttgart, 2008.
8. Organic Spectroscopy, LDS Yadav, Springer/Kluwer, 2005.
9. Organic Spectroscopic Analysis, R J Anderson, D J Bendell, P W Groundwater, RSC, Cambridge, 2004.
10. Mass spectrometry a foundation course, K Downard, RSC, Cambridge, 2004.
11. Structural analysis of organic compounds by combined application of spectroscopic studies, J T Clerc, E Pretsch, J Seibl, Elsevier, Amsterdam, 2001.
12. Biomolecular NMR Spectroscopy, J N S Evans, Oxford University, Oxford, 1995.
13. Modern NMR techniques and their Applications, Ed. A I Popov, Marcel Dekker, 1991.
14. Instrumental methods of analysis, H. H. Willard, L. L. Merritt, J. A. Dean and F.A. Settle, 7<sup>th</sup> edition, CBS Publishers and Distributors, 1989
15. Organic mass spectroscopy, K. R. Dass & E. P. James, IBH New Delhi, 1976.
16. The IR Spectra of complex molecules, Vols. I and II, L J Bellamy, Chapman and Hall, London, 1975.
17. Mass spectrometry of organic compounds, H. Budzkiewicz, Djerassi C. and D. H. Williams, Holden-Day New York, 1975.
18. Interpretation of organic mass spectra, F W McLafferty, W A Benjamin, London, 1973.
19. Organic spectroscopy, P. Laszlo and P. Stang, Harper & Row, New York, 1971.
20. Applications of absorption spectroscopy to organic compounds, J. R. Dyer, Prentice-Hall, New Delhi, 1969.
21. Interpretation of the UV spectra of natural products, A.I. Scott, Pergamon Press, Oxford,

1964.

**Ch-304-[OPEN ELECTIVE, NON-CHEMISTRY PAPER]**

## Ch- 304 OE: CHEMISTRY IN DAILY LIFE (OPEN ELECTIVE)

52 Hours

### UNIT-I

13hr

**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, disulphites,

**Artificial sweeteners:** aspartame, saccharin, dulcin, sucralose and sodium cyclamate.

**Flavours:** Vanillin, alkyl esters (fruit flavours) and monosodium glutamate.

**Artificial food colorants:** Coal tar dyes and non-permitted colours and metallic salts. Analysis of pesticide residues in food.

**Paints & Pigments:** White pigments (white lead, ZnO, lithopone, TiO<sub>2</sub>). Blue, red, yellow and green pigments. Paints and distempers: Requirement of a good paint. Emulsion, latex; luminescent paints. Fire retardant paints and enamels, lacquers. solvents and thinners for paints.

**Dyes:** Colour and constitution (electronic concept). Classification of dyes. Methods of applying dyes to the fabrics. A general study of azo dyes, Mordant brown, Congo red and methyl orange.

### UNIT II

**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.

**Composition of soil** – inorganic and organic components in soil-micro and macronutrients.

**Fertilisers:** Classification of Fertilizers- Straight Fertilizers, Compound/Complex Fertilizers, Fertilizer Mixtures. Manufacture and general properties of Fertilizer products- Urea and DAP.

### UNIT-III

**Carbohydrates:** Structure, function and Chemistry of some important mono and disaccharides.

**Vitamins:** Classification and Nomenclature. Sources, deficiency diseases and structures of Vitamin A, Vitamin B, Vitamin C, Vitamin D, Vitamin E & Vitamin K.

**Drugs:** Classification and nomenclature.

Structure and function of: *Analgesics* – aspirin, paracetamol;

*Anthelmintic drug:* mebendazole;

*Antiallergic drug:* Chlorpheniramine maleate,

*Antibiotics:* Penicillin V, Chloromycetin, Streptomycin.

*Anti-inflammatory agent:* Oxyphenbutazone,

*Antimalarials:* Primazaine phosphate & Chloroquine.

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

**Soaps & Detergents:** Structures and methods of use of soaps and detergents

#### UNIT IV

**Chemical Thermodynamics:** Concept of fugacity and free energy, Activity and activity coefficient, spontaneity of processes- entropy and free energy changes. Partial molar quantities, colligative properties, Le-Chatelier principle, phase equilibria. Enzyme catalysed reactions.

**Principles of Reactivity:** Basis kinetic concepts, rates of simple and complex chemical reactions, empirical rate equations. Temperature dependence of rates and activation parameters. Branched chain reactions – explosion limits. Oscillatory reactions.

**Corrosion:** Types and prevention, corrosion failure and analysis

**Chemical energy system** and limitations, principles and applications of primary & secondary batteries and fuel cell. Basics of solar energy, future energy storer.

**Polymers :** Types and classification of polymers. Source and general characteristics of natural and synthetic polymers. Typical examples of polymers used as plastics, in textiles, in electronic and automobile components, in the medical and aerospace materials. Problems of plastic waste management. Strategies for the development of environment friendly polymers.

#### **References**

1. B. K. Sharma: introduction to Industrial Chemistry, Goel Publishing, Meerut (1998)
2. Medicinal Chemistry by Ashtoush Kar.
3. Drugs and Pharmaceutical Sciences Series, Marcel Dekker, Vol. II, INC, New York.
4. Analysis of Foods – H.E. Cox: 13. Chemical Analysis of Foods – H.E.Cox and Pearson.
5. Foods: Facts and Principles. N. Shakuntala Many and S. Swamy, 4<sup>th</sup> ed. New Age International (1998)
6. Physical Chemistry – P I Atkins and J. de Paula – 7<sup>th</sup> Ed. 2002, Oxford University Press.
7. Handbook on Fertilizer Technology by Swaminathan and Goswamy, 6<sup>th</sup> ed. 2001, FAI.
8. Organic Chemistry by I. L. Finar, Vol. 1 & 2.
9. Polymer Science and Technology, J. R. Fried (Prentice Hall).

#### **Ch 305, 306, 307 and 308 Practicals**

**Inorganic, Organic, Physical and Analytical Chemistry practicals (I Sem Syllabus) (4 days a week, 4 hours a day)**

## FOURTH SEMESTER

### PHYSICAL CHEMISTRY SPECIALISATION Ch- 401 IC/PC: SOLID STATE CHEMISTRY (Common to physical and Inorganic chemistry)

52 Hours

#### UNIT-I

13h

##### **Electronic structure of solids**

Free electron theory of solids, results of free electron theory; limitations and success of free electron theory, Fermi distribution, Fermi sphere, volume of Fermi sphere, expression for energy levels in a solid, density of states, expression for the number of energy levels in a Fermi sphere.

##### **Electrical and Magnetic properties of Solids**

Electronic conductivity: Ohm's law, derivation of Ohm's law, Hall Effect, Band theory, Zone theory, Brillouin zones, K-space, k-vector, Significance of k-vector, Semiconductors: Energy bands in a semi conductor, temperature dependence of conductivity in metals and semi conductors, intrinsic and extrinsic semiconductors, Insulators; properties, Piezo and inverse Piezo electric effect. Pyroelectricity, Magnetic properties

#### UNIT-II

13h

##### **Heat Capacity of Solids**

Definition, Theories of heat capacity of solids: Dulong-petit, Einstein's theory, Debye Theory. Problems and their solution

##### **Defects in Solids**

Point defects, Schottky, Frenkel and interstitial, Line defects and Plane defects, Stacking faults and grain boundaries

##### **Superconductivity**

Superconductivity, BCS theory, Meisner effect, Type I and type II superconductors, Features of superconductors, Frolich diagram, Cooper pairs, Theory of low temperature superconductivity, *Junctions using superconductors*

##### **Phase Transition in Solids**

Definitions, Classification of phase transitions, First and second order phase transitions: *Martensitic transition, order-disorder transitions and spinodal decomposition*

#### UNIT-III

##### **Geometric Crystallography**

13h

Symmetry elements, Bravais lattices, Screw axes and glide planes, point groups, and space groups and nomenclature. Law of Interfacial angle (Euler's construction).

### **Diffraction theory and Single crystal X-ray diffraction**

X-rays, Bragg's law, assignment of lines, diffraction pattern of a primitive cubic lattice, space group extinctions, Scattering factor and structure factor, intensities from atomic positions for BCC and FCC lattices; Ewald's sphere of reflection, Reciprocal Lattice concept, Electron density function, Fourier synthesis, Fourier transform of the structure factor, Phase problem and Patterson synthesis.

### **UNIT-IV**

13h

#### **Experimental Methods**

Rotation, Oscillation, Weissenberg and Precession methods. Debye-Scherrer method (Powder method), Determination of lattice parameters from these methods.

#### **Electron diffraction**

Experimental technique, Wierl equation, Radial-Distribution method.

#### **Neutron diffraction**

Principle and Theory, advantages and uses.

### **SUGGESTED BOOKS**

1. Introduction to Solids, L. V. Azaroff, McGraw Hill Book Co., New York, 1960.
2. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Holt Saunders International Ltd. New York 1976.
3. Physical Chemistry, G. M. Barrow, McGraw Hill (2nd ISE) 1966.
4. An Introduction to X-ray Crystallography, M. M. Woolfson, Cambridge University Press-Vikas Publishing House, New Delhi 1980.
5. Principles of the Solid State, H. V. Kheer, Wiley Eastern Ltd., New Delhi 1993.
6. Vibrational Spectroscopy of Solids, P.M.A. Sherwood, Cambridge University Press, Cambridge, 1972.
7. Phase Transitions, C.N.R. Rao and K.J. Rao, McGraw Hill Book Co, Newyork 1978.
8. X-ray Structure determination: A practical guide, George H Stout and Lyle H Jenson, John Wiley & sons Newyork 1989.
9. Crystal structure analysis for chemists and biologists J.P Glusker, M.Lewis and M.Ross. Wiley-VCH 1994.

**Ch-402 PC: CHEMISTRY OF MACROMOLECULES AND ADVANCED  
PHOTOCHEMISTRY**

**52 Hours**

**UNIT-I**

**Molecular weight determinations:**

**13h**

Determination of molecular weight average by (i) osmotic pressure, Donnan membrane equilibrium, (ii) Light scattering, fundamental concepts, scattering from number of particles, Rayleigh scattering from solutions of macromolecules, scattering by macromolecules, (iii) Sedimentation velocity, (iv) Sedimentation equilibrium (v) density gradient sedimentation (vi) viscosity: specific viscosity, relative viscosity, intrinsic viscosity, Determination of molecular weight and size of macromolecules (vii) electrophoresis: isoelectric point, isoelectric focusing techniques and determination of molecular weight by electrophoresis technique.

Derivation of relevant expression in each of above experimental cases and use of these above methods in evaluation of shapes and confirmations of macromolecules

**UNIT-II**

**Thermodynamics of Polymer solution:**

**13h**

Partial molar and partial specific quantities, Chemical potential of macromolecular solution Gibbs-Duhem equation, concepts of second virial coefficient and excluded volume. Mathematical expressions for various models postulated for the shapes of macromolecules in solution; spheres, ellipsoid, long rod and flexible random coil

**Spectroscopic studies of Macromolecules:**

Determination of structure of macromolecules by UV-visible, Infrared, NMR, ESR, ORD and CD techniques

**UNIT-III**

**Mechanical properties**

**13h**

Structure property relationship of polymers: Strength, plastic deformation (rheology), physical state of polymers, chemical resistance, crystallinity, Mechanism of deformation, Methods of testing: Static testing-Poissons ratio, stress-strain curves. Transient testing and Impact testing

**Degradation, Stability and Environmental issues**

Thermal degradation, oxidative and UV-stability, chemical and hydrolytical stability, radiation effects.

Mechanical degradation, photodegradation, degradation by ultrasonic waves. Management of plastics in the environment. Recycling, Incineration and biodegradation.

**Advanced Photochemistry-I**

Born-Oppenheimer approximation, identification of molecular orbitals based on symmetry properties and symmetry elements, spectroscopic term symbols for molecules, direct product rule for assigning molecular symmetry from orbital symmetry, potential energy diagram for molecular oxygen electronic energy states in relation with the absorption spectrum, notation for excited states of organic molecules.

### **Molecular reaction dynamics**

Reactions in molecular beams, Potential energy surface for H + H<sub>2</sub> reaction, Theoretical calculation of activation energies of potential energy surfaces, Transmission co-efficient, Quantum mechanical tunneling, Reaction co-ordinate, Symmetry numbers and Statistical factors, Mean free path, Reaction rates and crosssections.

### **SUGGESTED BOOKS**

1. Chemical Kinetics, K. J. Laidler 3<sup>rd</sup> Edition (Mc-Graw Hill Inc.) New York,(2007).
2. Kinetics and Mechanism, Frost and R.G. Pearson (John-Wiley) New York,(1962).
3. Physical Chemistry, P. W. Atkins 7<sup>th</sup> Edn, (Oxford)(2004).
4. Introduction to Molecular Dynamics and Chemical Kinetics, G.D. Billing and Milkelson. (Wiley Interscience),(1996).
5. Organic Reaction Mechanism, R. K. Bansal (Mc- Graw Hill) New Delhi,1978.
6. Reaction Mechanism in Organic Chemistry, S.M. Mukheji, S.P.Singh and R.P. Kapoor (Mc. Millan India Ltd.,) Bangalore,(1978).
7. Catalysis, J. K. Kuriacose (McMillan India Ltd.,)(1991).
8. Text book of Polymer Science, F. W. Billmeyer (John-Wiley)1984.
9. Introductory polymer Chemistry, G. S. Misra (Wiley Eastern Ltd.,) New Delhi,1993.
10. Polymer Science, Gowrikar et al (Wiley Eastern Ltd.,) New Delhi,1990.
11. Introduction to Physical Organic Chemistry, R. D. Gilliom (Addison-Wesley) USA, 1970.
12. Physical Organic Chemistry, Reaction Rates Equilibrium and Mechanisms, L. P. Hammett, 2<sup>nd</sup> Edn, (Mc-Graw Hill Book. Co.)1970.
13. Biophysical Chemistry- Principles and Techniques, A. Upadyayay, K. Upadyayay, N. Nath (Himalaya Publishing House), Mumbai,1998.
14. Foundation of Chemical Kinetics, S. W. Benson (Mc-Graw Hill), New York,1960.
15. Comprehensive Chemical Kinetics, Vol-I, Banford and Tipper (Elsevier Publishing Co.,) New York1969.
16. Physical Chemistry, G. M. Barrow, 5<sup>th</sup> Edn., (Tata Mc-Graw Hill),1992.
17. Principles of Chemical Kinetics, J. E. House (Wm C Brown Publisher) Boston,1997.
18. Modern Physical Organic Chemistry-V. A. Eric and A.D. Dennis, University Science Books, USA,(2006).
19. Physical Chemistry, R. J. Silbey, R. A. Alberty and M. G. Bawendi; 4<sup>th</sup>Edn. Wiley (2009)
20. Molecular Reaction Dynamics, Hardy Levin and R. B. Bernstein, Oxford University Press, New York(1974).

## Ch-404 IC/ PC: INORGANIC SPECTROSCOPY

(Common to Inorganic and Physical Chemistry)

52 Hours

### UNIT-I

#### **Vibrational spectroscopy**

13h

Vibrational spectra of diatomic, linear and bent triatomic,  $AB_3$ ,  $AB_4$ ,  $AB_5$  and  $AB_6$  molecules, spectra of metal complexes: Ammine, amido, Nitro, Nitrito, lattice water, aquo and hydroxo, carbonato, nitrate, sulphato and other acido complexes, cyano and nitrile complexes, cyanato and thiocyanato complexes, mono and multinuclear carbonyl complexes, nitrosyls, phosphines and arsines, ambidentate ligands, ethylenediamine and diketonato complexes.

#### **Raman spectroscopy**

Resonance Raman Spectroscopy, Nonlinear Raman effects-Stimulated, hyper and inverse types, coherent anti-stokes Raman scattering (CARS) Lasers and their use in Raman spectroscopy. Resonance Raman spectrum of  $K_2CrO_4$  and complexes with peroxide linkage.

### UNIT-II

#### **Photoelectron spectroscopy**

13h

Basic principles- photoelectric effect, Koopman's theorem, XPS and UPS, spin-orbit coupling in core level spectra, applications of core level spectra-ESCA, chemical shift, Valence level spectra-  $n$ ,  $\sigma$  and  $\pi$  bands, Auger electron spectroscopy and applications, Electron energy loss spectroscopy- basic principles and applications  
Applications to the study of solids.

#### **Mossbauer spectroscopy**

Basic principles, isomer shift, quadrupole splitting and magnetic hyperfine interactions, application to the study of bonding and structures of  $Fe^{2+}$  and  $Fe^{3+}$  compounds,  $Sn^{2+}$  and  $Sn^{4+}$  compounds

### UNIT-III

#### **Electron spin resonance spectroscopy**

13h

Basic principles, the position of ESR absorption, significance of 'g' factor, determination of 'g' factor. Electron-nucleus coupling (Hyperfine splitting). ESR spectrometer, electron-electron coupling, double resonance in ESR, ENDOR, ELDOR.

Interpretation of ESR spectra and structure elucidation of organic radicals using ESR spectroscopy. Spin density and McConnell relationship. Spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, zero/non-zero field splitting, Kramer's degeneracy,

application to transition metal complexes (having one to five unpaired electrons) including biological molecules and inorganic free radicals such as  $PH_2$ ,  $F_2$  and  $BH_2$ .

#### **X-ray absorption spectroscopy**

Near edge measurements and EXAFS

## UNIT-IV

### **NMR spectroscopy of inorganic molecules**

13h

Proton NMR spectra of metal hydride complexes

NMR spectra of nuclei other than hydrogen:  $^{19}\text{F}$ ,  $^{31}\text{P}$ ,  $^{11}\text{B}$  NMR spectra of simple compounds,

Proton/hydride interactions with  $^{103}\text{Rh}$ ,  $^{183}\text{W}$ ,  $^{195}\text{Pt}$  and  $^{207}\text{Pb}$  in metal complexes/organometallic compounds,

Solid State NMR.

### **NQR spectroscopy**

NQR isotopes, electric field gradients, Nuclear Quadrupole coupling constants, Experimental techniques and applications

### **SUGGESTED BOOKS**

1. Physical methods in Inorganic Chemistry, R.S. Drago, Affiliated East West Press Pvt. Ltd., New Delhi 1965.
2. Infrared spectra of Inorganic and Coordination Compounds, K. Nakamoto, Wiley Interscience, New York 1970.
3. Vibrational Spectroscopy: Theory and Applications, D.N. Sathyanarayana, New Age International Publishers, New Delhi 2000.
4. Electronic Absorption Spectroscopy and Related Techniques, D.N. Sathyanarayana, Universities Press, Bangalore 2001.
5. Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR, D.N. Sathyanarayana, I.K. International Publishing House Pvt.Ltd., New Delhi 2009.

## **PHYSICAL CHEMISTRY PRACTICALS**

(4 days a week, 4 hours a day)

### **Ch-405 : Kinetics and Thermodynamic Experiments**

1. Determination of order of the reaction for the hydrolysis of methyl acetate and evaluation of activation parameters
2. Kinetics of oxidation of glycine by chloramines-T, determination of order with respect to glycine
3. Degree of hydrolysis of urea-hydrochloride from the study of acid hydrolysis of methyl acetate.
4. Determination of mean-ion activity co-efficient of HCl and the study of the effect of ionic strength on the activity co-efficient of  $\text{Ag}^+$  ions.
5. Determination of the free energy change of a cell reaction.
6. Study of acetone-iodine reaction-determination of order with respect to each reactant by ratio variation method.
7. Kinetics of decomposition of  $\text{H}_2\text{O}_2$ - effect of catalyst and promoter.
8. Study of decomposition of diacetone alcohol using dilatometer- Evaluation of catalytic coefficient of  $\text{OH}^-$  ions,  $E_a$  and thermodynamic parameters.
9. Kinetics of oxidation of indigo carmine by chloroamine-T-spectrophotometrically and determination of  $E_a$  and thermodynamic parameters.
10. Determination of catalytic efficiency of  $\text{RuCl}_3$  for the reaction between a primary amine and CAT.

#### **Ch-406 : Conductometric and Potentiometric experiments**

1. Study of kinetics of hydrolysis of t-butyl chloride by conductivity method, determination of rate constant, energy of activation and thermodynamic parameters
2. Study of the complex formation and determination of the stability constant of silver ammonia complex.
3. Determination of solubility of silver halides in a mixture.
4. Determination of acid and base dissociation constants of an amino acid and hence its isoelectric point by pH metry.
5. Determination of pKa values of a poly basic acid potentiometrically using quinhydrone electrode.
6. Determination of pKa values of a poly basic acid pHmetrically.
7. Titration of ferrous ammonium sulphate against potassium dichromate using a bimetallic electrode.
8. Conductometric titrations of Thorium nitrate with potassium tartrate.
9. Conductometric titrations of Potassium iodide with mercuric perchlorate
10. Conductometric titrations of acetic acid, monochloro acetic acid and trichloro acetic acid with strong alkali.

#### **Ch-407 : Kinetics and Instrumental Methods**

1. Study of the effect of dielectric constant using methanol on the kinetics of the reaction between a primary amine and CAT.
2. Study of effect of salt (ionic strength) on the kinetics of the reaction between potassium persulphate and potassium iodide.
3. Kinetics of autocatalytic reaction between potassium permanganate and oxalic acid.
4. Absorption spectrum of a conjugated dye and verification of quantum mechanics of particle in one dimensional box
5. Spectral interpretation for structure elucidation of simple organic compounds (-COOH, -OH, -NH<sub>2</sub>, and -Cl) by FT-IR.
6. Powder diffraction pattern of simple salt and determination of lattice type and the parameters.
7. Evaluation of cell parameters from rotational photograph.
8. Demonstration of fluorescence of solution of anthracene in benzene with respect to UV-visible absorption spectra.
9. To construct the phase diagram of a three component systems (CHCl<sub>3</sub>-acetic acid-water).
10. Determination of the relative strength of monochloroacetic acid(4N) and trichloroacetic acid(4N) by the study of kinetics of hydrolysis of methyl acetate.

#### **Ch-408 : Electrochemical and Instrumental methods**

1. Differential potentiometric titrations of weak acid against strong base
2. Differential potentiometric titrations of a mixture of strong and weak acids against strong base
3. Determination of hydrolysis constant of aniline hydrochloride conductometrically
4. Determination of equivalent conductance of a weak electrolyte (acetic acid) at infinite dilution following Kohlrausch law.
5. Spectrophotometric determination of indicator constant (bromophenol blue) 6.

6. Determination of stability constant of a complex formed between salicylic acid and ferric ion by variation of pH.
7. Determination of corrosion rate of Zn in NaOH by weight loss method.
8. Identification of metal ions in a mixture polarographically
9. Determination of molecular weight of a polymer by viscosity method.
10. Study of the redox behavior of  $K_4Fe(CN)_6/K_3Fe(CN)_6$

### SUGGESTED BOOKS

1. Findlays practical physical chemistry revised by P. B. Levitt, Longman's London(1966).
2. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International Edn.(1966).
3. Advanced Practical Physical Chemistry by J. B. Yadav, Goel Publications Meerut(1988).
4. Senior Practical Physical Chemistry by B. C. Kosla, Simla Printers New Delhi(1987).
5. Experimental Physical Chemistry by Daniel et al., McGraw Hill, New York(1962).
6. Practical Physical Chemistry by A.M James and P. E. Pritchard, Longman's Group Ltd(1968)
7. Experimental Physical Chemistry by V.D.Atavale, and Parul Mathur, New Age International, New York (2001)
8. Physical Chemistry Laboratory Principles and Experiments by H.W.Salberg, J.L. Morrow, S.R.Cohen and M.E. Green, Mac millam Publishing Co. New York
9. Experimental Physical Chemistry by Wilson, Newcombe & others, Pergamon Press, New York(1962)
10. Practicals in Physical Chemistry. A modern Approach by P.S.Sindhu, Macmillan Publishers, Delhi, 2006
11. Experimental Physical Chemistry by R. C. Behra and B Behra, Tata McGraw, New Delhi (1983).

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