

# Shivaji University, Kolhapur

# Department of Chemistry

# M.Sc. Part-II Chemistry Syllabus as Per New CBCS PATTERN

(Inorganic, Organic, Physical and Analytical)

To be implemented from June- 2020-2021

Applicable for University Department and Affiliated Colleges PG Center

# M. Sc. Programme structure (CBCS PATTERN)

# M. Sc. Part – I (Inorganic, Organic, Physical, Analytical, Applied and Industrial Chemistry)

	Course code	Paper		Title of course	
		No.			
	CC-101	Ι	CH.1.1	Inorganic Chemistry - I	All courses are
CGPA	CC-102	II	CH.1.2	Organic Chemistry - I	compulsory.
	CC-103	III	CH.1.3	Physical Chemistry - I	
	CC-104	IV	CH.1.4	Analytical Chemistry - I	
	CCPR-105		CHP.1.1	Practical- I	
Non-	AEC -106				
CGPA					

# Semester I

	Course code	Paper		Title of course	
		No.			
	CC-201	V	CH.2.1	Inorganic Chemistry – II	All courses are
	CC-202	VI	CH.2.2	Organic Chemistry – II	compulsory.
CGPA	CC-203	VII	CH.2.3	Physical Chemistry – II	
	CC-204	VIII	CH.2.4	Analytical Chemistry - II	
	CCPR-205		CHP.2.1	Practical -II	
Non-	SEC - 206				
CGPA					

# M. Sc. Part – II (Inorganic Chemistry)

# Semester III

	Course code	Paper No.		Title of course	
	CC-301	IX IX	ICH 3.1	Inorganic Chemical Spectroscopy	Compulsory course
CGPA	CCS-302	X	ICH 3.2	Coordination Chemistry - I	Compulsory course
Non-	CCS-303	XI	ICH 3.3	Nuclear Chemistry	Compulsory course
CGPA	DSE-304(A)	XII(A)	ICH 3.4(A)	Organometallic and	Choose any one
				Bioinorganic Chemistry	
	DSE-304(B)	XII(B)	ICH 3.4(B)	Selected Topics in Inorganic	Choose any one
				Chemistry	
	CCPR-305		ICHP 3.1	Practical -III	Compulsory course
	AEC-306				
	EC(SWMMOOC)-				
	307				

	Course code	Paper		Title of course	
		No.			
	CC-401	XIII	ICH 4.1	Instrumental Techniques	Compulsory course
	CCS-402	XIV	ICH 4.2	Coordination Chemistry II	Compulsory course
CGPA	CCS-403	XV	ICH 4.3	Chemistry of Inorganic Materials	Compulsory course
	DSE-404(A)	XVI(A)	ICH 4.4(A)	Energy and Environmental	Choose any one
				Chemistry	
	DSE-404(B)	XVI(B)	ICH 4.4(B)	Radiation Chemistry	Choose any one
	CCPR-405		ICHP 4.1	Practical –IV	Compulsory course
Non-	SEC-406				
CGPA	GE-407				

# M. Sc. Part – II (Organic Chemistry)

# Semester III

	Course code	Paper		Title of course	
		No.			
	CC-301	IX	OCH 3.1	Organic Reaction Mechanism	Compulsory course
	CCS-302	Х	OCH 3.2	Advanced Spectroscopic	Compulsory course
CGPA				Methods	
	CCS-303	XI	OCH 3.3	Advanced Synthetic Methods	Compulsory course
	DSE-304(A)	XII(A)	OCH 3.4(A)	Drugs and Heterocycles	Choose any one
	DSE-304(B)	XII(B)	OCH 3.4(B)	Polymer Chemistry	Choose any one
	CCPR-305		OCHP 3.1	Practical –III	Compulsory course
Non-	AEC-306				
CGPA	EC(SWMMOOC)-				
	307				

	Course code	Paper		Title of course	
		No.			
	CC-401	XIII	OCH 4.1	Theoretical Organic Chemistry	Compulsory course
	CCS-402	XIV	OCH 4.2	Stereochemistry	Compulsory course
CGPA	CCS-403	XV	OCH 4.3	Chemistry of Natural Products	Compulsory course
	DSE-404(A)	XVI(A)	OCH 4.4(A)	Applied Organic Chemistry	Choose any one
	DSE-404(B)	XVI(B)	OCH 4.4(B)	Bioorganic Chemistry	Choose any one
	CCPR-405		OCHP 4.1	Practical –IV	Compulsory course
Non-	SEC-406				
CGPA	GE-407				

# M. Sc. Part – II (Physical Chemistry)

# Semester III

	Course code	Paper		Title of course	
		No.			
	CC-301	IX	PCH 3.1	Advanced Quantum Chemistry	Compulsory course
	CCS-302	Х	PCH 3.2	Electrochemistry	Compulsory course
CGPA	CCS-303	XI	PCH 3.3	Molecular Structure – I	Compulsory course
	DSE-304(A)	XII(A)	PCH 3.4(A)	Solid State Chemistry	Choose any one
	DSE-304(B)	XII(B)	PCH 3.4(B)	Advanced Chemical Kinetics	Choose any one
	DSE-304(C)	XII(C)	PCH 3.4(C)	Radiation and Photochemistry	
	CCPR-305		PCHP 3.1	Practical –III	Compulsory course
Non-	AEC-306				
CGPA	EC(SWMMOOC)-				
	307				

	Course code	Paper		Title of course	
		No.			
	CC-401	XIII	PCH 4.1	Thermodynamics and Molecular	Compulsory course
				Modeling	
CGPA	CCS-402	XIV	PCH 4.2	Chemical Kinetics	Compulsory course
	CCS-403	XV	PCH 4.3	Molecular Structure - II	Compulsory course
	DSE-404(A)	XVI(A)	PCH 4.4(A)	Surface Chemistry	Choose any one
	DSE-404(B)	XVI(B)	PCH 4.4(B)	Chemistry of Materials	Choose any one
	DSE-404(B)	XVI(C)	PCH 4.4(C)	Biophysical Chemistry	
	CCPR-405		PCHP 4.1	Practical –IV	Compulsory course
Non-	SEC-406				
CGPA	GE-407				

# M. Sc. Part – II (Analytical Chemistry)

	Course code	Paper No.		Title of course	
	CC-301	IX	ACH 3.1	Advanced Analytical Techniques	Compulsory course
CGPA	CCS-302	Х	ACH 3.2	Organo Analytical Chemistry	Compulsory course
	CCS-303	XI	ACH 3.3	Electroanalytical Techniques in Chemical Analysis	Compulsory course
	DSE-304(A)	XII(A)	ACH 3.4(A)	Environmental Chemical Analysis and Control	Choose any one
	DSE-304(B)	XII(B)	ACH 3.4(B)	Recent Advances in Analytical Chemistry	Choose any one
	CCPR-305		ACHP 3.1	Practical –III	Compulsory course
Non-	AEC-306				
CGPA	EC(SWMMOOC)- 307				

# Semester III

	Course code	Paper		Title of course	
		No.			
	CC-401	XIII	ACH 4.1	Modern Separation Methods in	Compulsory course
				Analysis	
CGPA	CCS-402	XIV	ACH 4.2	Organic Industrial Analysis	Compulsory course
	CCS-403	XV	ACH 4.3	Advanced Methods in Chemical	Compulsory course
				Analysis	
	DSE-404(A)	XVI(A)	ACH 4.4(A)	Industrial Analytical Chemistry	Choose any one
	DSE-404(B)	XVI(B)	ACH 4.4(B)	Quality Assurance and	Choose any one
				Accreditation	
	CCPR-405		ACHP 4.1	Practical –IV	Compulsory course
Non-	SEC-406				
CGPA	GE-407				

# M.Sc. Part-II, (Sem-III and IV) Inorganic Chemistry

# **SEMESTER-III**

Paper No-IX, ICH 3.1	: INORGANIC CHEMICAL SPECTROSCOPY
Paper No. –X, ICH 3.2	: COORDINATION CHEMISTRY – I
Paper No. –XI, ICH 3.3	: NUCLEAR CHEMISTRY
ELECTIVE PAPERS	
Paper No. –XII(A), ICH 3.4(A)	) : ORGANOMETALLIC AND BIOINORGANIC
	CHEMISTRY
Paper No. $-XII(B)$ , ich $3.4(B)$	: SELECTED TOPICS IN INORGANIC
	CHEMISTRY
Practical Course	: ICHP-V and ICHP- VI

# **SEMESTER-IV**

Paper No. –XIII, ICH 4.1	: INSTRUMENTAL TECHNIQUES.
Paper No. – XIV, ICH 4.2	: COORDINATION CHEMISTRY-II
Paper No. –XV, ICH 4.3	: CHEMISTRY OF INORGANIC MATERIALS
ELECTIVE PAPERS	
Paper No. –XVI(A), ICH 4.4(A)	: ENERGY AND ENVIRONMENTAL CHEMISTRY
Paper No. –XVI(B), ICH 4.4(B)	: RADIATION CHEMISTRY
Practical Course	: ICHP - VII and ICHP-VIII

# M.Sc. Part-II (Sem- III) Inorganic Chemistry

# Paper No. –IX, ICH 3.1: Inorganic Chemical Spectroscopy

# **Unit I: Molecular Symmetry and Group Theory**

Introduction to Symmetry, Symmetry operations, Symmetry elements, Point group and its classification (Cn-type, Dn-type, Special-type), Schoenflies symbol for point groups, Determination of point group for AB<sub>2</sub> (Bent), AB<sub>3</sub> (Trigonal pyramid), AB<sub>3</sub> (Trigonal Planar), AB<sub>4</sub> (Square planar), AB<sub>5</sub> (Trigonalbipyramidal), AB<sub>6</sub> (Octahedral), CO<sub>2</sub>, HCl, CO, Ortho-, meta- & para-disubstituted benzene molecules. Symmetry and dipole moment of molecule, Symmetry and optical activity, Group and its Properties, Group multiplication table, Matrix representation of symmetry elements, Reducible and Irreducible representations, Character of a representation (character of matrix), Properties of Irreducible representation, Great orthogonally theorem (without proof) and its importance, Construction of character table for C<sub>2v</sub>& C<sub>3v</sub> point groups, Mulliken symbolism rules for irreducible representations & its illustrations, Direct product, Standard reduction formula.

# **Unit II: IR and Raman Spectroscopy**

A) Infrared spectroscopy: The vibrating diatomic molecule, The simple harmonic oscillator, The anharmonic oscillator, The diatomic vibrating rotator, Vibration- rotation spectrum of carbon monoxide, Breakdown of Born-Oppenheimur approximation, The vibration of polyatomic molecules, Overtones and combination frequencies, The influence of rotation of the spectra of polyatomic molecules, Techniques and Instrumentation, Applications.

B) Raman spectroscopy: Classical and Quantum theory, Pure rotational Raman Spectra, vibrational Raman spectra, Rule of mutual exclusion, Overtone and combination vibrations, Rotational fine structure, Outline of technique and instrumentation, Applications.

Modes of vibrations, Selection Rules for Infrared and Raman Spectra, Normal modes of vibrations in AB<sub>2</sub> (Linear/Bent), AB<sub>3</sub>, AB<sub>4</sub>, AB<sub>5</sub>, Octahedral AB<sub>6</sub> molecules with factors affecting band frequencies.

#### **Unit III: Mass Spectroscopy:**

Basic principle, Instrumentation, Electron-impact Induced and Fast Atom Bombardment (FAB) spectrometry, qualitative and semiquantitative theories including QET, concept of metastable ions transitions, Stevensons's rules. Applications to metal compounds containing carbonyl, alkyl, cyclopentadienyl and acetylacetonate.

# Unit IV: A) NMR Spectroscopy:

Principle Instrumentation of NMR, the chemical shift, mechanism of electron shielding and factors contributing to the magnitude of chemical shift. Local & remote effect, spin-spin splitting, applications of spin coupling to structural determination, double Resonance techniques. The contact and Pseudo contact shifts Factors affecting nuclear relaxation, an overview of NMR of metal nucleus with emphasis on <sup>195</sup>Ag &<sup>119</sup>Sn NMR, applications of solid-state NMR technique.

15 Hrs.

15 Hrs.

# 8 Hrs

# **B)** X-ray Photo electron Spectroscopy (XPS)

Introduction and basic theory, Instrumentation, sample selection and preparation, spectral analysis, Ar ion sputtering technique and applications of XPS.

#### **Reference Books:**

- 1. K. Burger, Coordination Chemistry-experimental methods, Butterworth's
- 2. R. Drago: Physical method in Inorganic Chemistry, DUSAP.
- 3. Hill & Day advanced methods in Inorganic Chemistry, J.Weily
- 4. F.A. Cotton, chemical application of group theory, Weily eastern
- 5. Figgis, Introduction to ligand field theory field
- 6. Schaefer & Gilman: Basic principles of ligand field Theory, J. Wiely
- 7. P.R. Backer: Molecular symmetry and Spectroscopy A.P.
- 8. Ferraro Ziomeek, Introduction to Group theory, plenum
- 9. Scotland Molecular symmetry DVN
- 10. Dorian: symmetry in Chemistry EWAP
- 11. Hall: Group theory and symmetry in Chemistry MGLt
- 12. Nakamoto Infrared R Raman Spectra of Inorganic & Coordination compounds J.Weily
- 13. Nakanisha: Spectroscopy and structure J. Weily
- 14. Ferroro: Metal ligand and related vibrations
- 15. CNR Rao Spectroscopy in Inorganic Chemistry Vol I, II, III
- 16. Durie: vibrations spectra and structure Vol. I to IV, Elsevier
- 17. Dudd, chemical Spectroscopy Elsevier
- 18. Popel: H.N.M.R. Spectroscopy J.Weily
- 19. R.J. Abraham, J.Fisher and P Loftus Wiley Introduction to NMR spectroscopy.
- 20. P.K. Bhattacharya: Group Theory & Its Chemical Applications
- 21. K.V. Reddy: Symmetry & spectroscopy of Molecules.
- 22. M. R. Litzow and T R Spelding, Mass Spectroscopy of Inorganic & Organometallic Compounds, Elsevier,73

# Paper No.-X, ICH 3.2: Coordination Chemistry-I

# Unit I: Metal-ligand bonding:

Crystal Field Theory: Splitting of d-orbital in tetragonal, square planar and trigonal bipyramid complexes. CFSE-factors affecting the magnitude of 10 Dq-evidence for crystal field stabilization, tetragonal distortion from octahedral symmetry, John teller effect, nephelauxetic effect. CFSE and their uses, factors affecting CFSE, Limitations of crystal field theory. M.O. theory for octahedral, tetrahedral and square planar complexes with and without  $\pi$ -bonding.

### **Unit II: Electronic spectra of Transition Metal complexes:**

Determining the Energy terms, Spin-orbit (L-S) coupling scheme, Hund's rule, Derivation of the term symbol for a d<sup>1</sup> to d<sup>9</sup> configuration, Electronic spectra of transition metal complexes – Laporte 'orbital' selection rule, spin selection rule. Orgel diagrams for octahedral metal complexes. Racah parameters, calculations of 10 Dq, B and  $\beta$  parameters for octahedral complexes of cobalt and nickel, Tanabe-Sugano diagrams for octahedral complexes, Charge

# 15 Hrs.

15 Hrs.

transfer spectra, Selection rule and charge transfer spectra

#### Unit III: Magnetic properties of Transition metal complexes: :

Types of magnetic behaviour, origin of paramagnetism, Spin-orbit interaction, Lande interval rule, Diamagnetism, Pascal constants, Ferromagnetism and antiferromagnetism of metal complexes; temperature dependent paramagnetism, Van Vleck's equation, Its derivation and applications, magnetic anisotropy, anamoulous magnetic moment, Quenching of orbital moment, Spin orbit coupling and magnetic moment, Determination of magnetic susceptibility. Spins crossover phenomenon

# Unit IV: Mixed Ligand complexes

Stabilities of ternary complexes, Dynamics of formation of ternary complexes reaction of Coordination ligand in ternary complexes, Mimicking reactions in biological systems, enzyme models, Amino acids ester hydrolysis, peptide synthesis & hydrolysis, Decarboxylation of  $\beta$ -keto acids, Applications of mixed ligand complexes in catalysis.

# **Reference Books:**

- 1. Jones: Elementary Coordination Chemistry. J. Weily
- 2. Graddon: Introduction to Coordination Chemistry. J. Weily
- 3. Drago: Physical methods of Inorganic Chemistry. J. Weily.
- 4. Graddon: Introduction to coordination Chemistry, Parasmom
- 5. Lewis and Wilkins: Coordination Chemistry. J. Weily
- 6. Msrtel: Coordination Chemistry Vol I, II VNR
- 7. Earnshaw: Introduction to Magneto Chemistry
- 8. Mabbs & Machin Magnetism & transition metal complexes Chamman hall
- 9. Calvin, Magnetic properties of transition metal complexes.
- 10. L.N. Maley: Magneto Chemistry
- 11. Datta & Shymlal: Elements of Magneto Chemistry
- 12. Martel & Taqui Khan: homogeneous catalysis with metal complexes Vol.I & II AP.
- 13. James E. Huheey: Inorganic Chemistry Principles of Structure and reactivity, Harber and Row, Publishers Inc. New York 1972.
- 14. K.P. Purcell & J.C. Kote: An Introduction to Inorganic Chemistry Holt Sounders, Japan 1980.
- 15. William L. Jolly: Modern Inorganic Chemistry, Mecgrow Hill USA, 1984
- 16. F.A. Cotton & R.G. Wilkinson: Advanced Inorganic Chemistry

15 Hrs

# Paper No. –XI, ICH 3.3 : Nuclear Chemistry

# UNIT-I: Systematic of alpha, beta and gamma decays

Alpha decay, energy curve, spectra of alpha particles, Giger-Nuttal law, theory of alpha decay, penetration of potential barrier, beta decay, range of energy relationship, beta spectrum, sergeants curve, Fermi theory of beta decay, matrix elements, allowed and forbidden transitions, curie plots, gamma decay, Nuclear energy levels, selection rule, isomeric transitions, Internal conversion, Auger effect

#### **UNIT-II: Nuclear Structure and Stability**

Binding energy, empirical mass equation, The nuclear models, the liquid drop model, Single particle shell model, Fermi gas model & collective/lunified nuclear model, nuclear spin, parity & magnetic moments of odd mass number nuclei and numerical.

#### Unit III: Nuclear reactions and Nuclear fission

Introduction, Production of projectiles, nuclear cross section, nuclear dynamics, threshold energy of nuclear reaction, Coulomb scattering, potential barrier, potential well, formation of a compound nucleus, Nuclear reactions, direct Nuclear reactions, heavy ion induced nuclear reactions, photonuclear reactions.

Liquid drop model of fission, fission barrier and threshold, fission cross section, mass energy and charge distribution of fission products, symmetric and a symmetric fission, decay chains and delayed neutrons

# UNIT-IV: Reactor Theory and Applications of Radioactivity

Nuclear fission as a source of energy, Nuclear chain reacting systems, critical size of a reaction, research reactors, graphite moderated, heterogeneous, enriched uranium reactors, light water moderated, heterogeneous, enriched uranium reactors, water boilers enriched aq. Homogeneous reactors, Thermonuclear reactors, gamma interactions, shielding and health protection. Reactors in India.

Tracer technique in the field of analytical chemistry structure determination elucidation of reaction mechanism, isotopic dilution analysis, neutron activation analysis applications in biological, medical, industrial fields, Age determination.

# **Reference Books**

1. Friedlander, Kennedy and Miller, Nuclear and Radio Chemistry: John Wiley

- 2. B. G. Harvey, Nuclear Chemistry
- 3. Hassinsky: Translated by D. G. Tuck, Nuclear Chemistry and its application: Addison Wiley
- 4. B.G. Harvey, Introduction to Nuclear Physics and Chemistry
- 5. Maeclefort: Nuclear Chemistry: D. Van Nostrand
- 6. An N. Nesmeyannoy: Radiochemistry: Mir
- 7. Jacobs et al: Basic Principles of nuclear Science and Reactors, V. Nost & EWAP
- 8. N. Jay: Nuclear Power Today Tomorrow: ELBS
- 9. Kenneth: Nuclear Power Today, Tomorrow: ELBS
- 10. Essentials of Nuclear Chemistry, W. J. Arnikar, John Wiley
- 11. Nuclear and Radiation Chemistry: B. K. Sharma, Krishna Publication

#### 15 Hrs

# 15 Hrs

15 Hrs

12. A Introduction to Nuclear Physics: R. Babber. And Puri.

13. Essential of Nuclear Chemistry by H. J. Arnikar

# Paper No. –XII(A), ICH 3.4(A) : Organometallic and Bioinorganic Chemistry

# **Unit I: Organotransition Metal Chemistry:**

Alkyls and Aryls of Transition Metals: Types, routes of synthesis, stability and decomposition pathways of alkyls and aryls of transition metals. Organocopper in Organic synthesis. Compounds of Transition Metal -Carbon Multiple bonds: Alkylidenes, alkylidynes, low valent carbenes and carbynes-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on ligands, role in organic synthesis.

# **Unit-II: Transition Metal Pi-complexes**

Carbon multiple bonds. Nature of bonding, structural characteristics & synthesis, properties of transition metal Pi-Complexes with unsaturated organic molecules, alkenes alkynes, allyl, diene, dienyl, arene and trienyl complexes. Application of transition metal, organometallic intermediates in oraganic synthesis relating to nucleophilic and electrophilic attack on ligands, role in organic synthesis.

# **Unit III: Metal Compounds in Medicine**

Medicinal use of metal complexes as antibacterial, anticncer, use of cis-platin as antitumor drug, antibiotics & related compounds. Metal deficiency and disease, iron deficiency, zinc deficiency and copper deficiency, Metal used for dignosis and chemotherapy with particular reference to anti cancer drugs. Chelate therapy, chemotherapy with compounds of some non essential elements; platinum complexes in cancer therapy. Antiviral activity of metal complexes. Gold containing drugs used in the therapy of Rheumatic-Arthritis, Gold complexes as anticancer drug. Lithium in psycho pharmacological drugs. Antimicrobial agents

# **Unit-IV: Oxygen Transport and Storage**

Heme proteins and oxygen uptake, structure and functions of haemoglobin, myoglobin, hemocyanins & hemerythrin. Perutz mechanism for structural changes in porphyrin ring system, Oxygenation and deoxygenation. Oxygen adsorption isotherm and cooperativity, physiological significance of haemoglobin, role of globin chain in gaemoglobin, Cyanide poisoning and treatment.

# **Reference Books**

- 1. Yamamoto, Organo Transition Metal Chemistry, Wiley (1986).
- 2. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals (4th edn.), John Wiley (2005).
- 3. A. J. Pearson. Metallo-Organic Chemistry, John Wiley & Sons (1985).
- 4. M. Bochmann. Organometallics-I Complexes with Transition Metal-Carbon σ-Bonds,

15 Hrs

15 Hrs

# 15 Hrs

Oxford Chemistry Primers (1994).

- 5. Principles of Biochemistry, A. L. Lehinger, Worth Publications.
- 6. Biochemistry, L. Stryer, W. H. Freeman
- 7. Biochemistry, J. David Rawn, Neil Patterson.
- 8. Biochemistry, Voet and Voet, John Wiley.
- 9. Outlines of Biochemistry, E. E. Conn and P. K. Stumpt, John Wiley.
- 10. D. F. Shriver, P. W. Atkins and C. H. Langford, Inorganic Chemistry, Oxford Univ. Press, 1990.
- 11. J. E. Huheey, E. A. Keiter and R.L. Keiter Inorganic Chemistry, Principles of Structure and Reactivity, Pearson Education, 2004.
- F. A. Carey G. Wilkinson, C. A. Murillo and M. Bochmann, Advanced Inorganic Chemistry, Wiley Interscience, 2003
- 13. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, Univ. Science Books, 1994.
- 14. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life (An introduction and Guide), John Wiley & Sons, 1994.
- 15. Zagic: Microbial Biogeochemistry, Academic press

# Paper No. –XII(B), ICH 3.4(B) : Selected Topics in Inorganic Chemistry

# **UNIT-I: Catalysis**

Basic principals, thermodynamic and kinetic aspects, industrial requirements, classification, theories of catalysis, homogeneous and heterogeneous catalysis. Introduction, types & characteristics of substrate-catalyst interactions, kinetics and energetic aspects of catalysis, selectivity, stereochemistry, orbital symmetry and reactivity. Catalytic reactions of coordination and Organometallic compounds including polymerization activation of small molecules, addition to multiple bonds, hydrogenation, Zeigler-Natta polymerization of olefins, monsanto acetic acid process.

#### **UNIT-II: Coordination Polymers**

Natural polymers and reactions yielding coordination polymers. Synthesis of coordination polymers. Use of polymeric ligands in synthesis of coordination polymers. Metal coordination polymers. Silicon polymers. Organosilicon polymers: synthesis and their uses

# UNIT-III: Non-conventional sources of energy

a) Alternate source of energy

Solar sources: Photochemical methods, thermodynamic efficiency of energy conversion, energy from solar radiations, transition metal complexes for energy production, solar hydrogen system, photochemical processes at semiconductors electrodes, photo galvanic and Photovoltaic cells based on Inorganic photochemical systems.

b) Geothermal energy

- c) Energy from biogas sources, biodiesel,
- d) Tidal wind sources

# 15 Hrs

# 15 Hrs

e) Energy from fission and fusion reaction.

# **Unit-IV Supramolecular Chemistry:**

Concepts and principles, Host-Guest Chemistry, Non-covalent bonds, crown ethers, cryptands and their metal complexes, Molecular recognition for different types of molecules, spherical recognition, Tetrahedral recognition, cooperativity and multivalency, Design and synthesis of co-receptor molecules and multiple recognition, supramolecular reactivity and catalysis, supramolecular devices, supramolecular photochemistry

# **Reference Books**

- 1. Heterogeneous catalysis 2nd edn. Bond C. Chapman all (1987).
- 2. The application & Chemistry of catalysis by suitable transition metal complexes Parashall. W. Weily N. 1980.
- 3. Homogeneous transition metal catalysis, A general art, Masters C. Chapman and Hall, London 1981.
- 4. Introduction to the principles of heterogeneous catalysis, Thomas J.M., Thomas W.J. Academic press N.Y. 1967
- 5. Inorganic polymers: Mark J.F., Allock H.R. West, Prentice hall
- 6. Inorganic polymers: Ring N.H., Academic Press N.Y. 1978
- 7. The Inorganic heterocyclic chemistry of sulphur, nitrogen, phosphorous, Heal A.G. Acta, Press N.Y. 1980.
- 8. Solar energy Principles of thermal collections and storage, Sukhatme S.P., Tata Macgrow Hill New Delhi 1984.
- 9. Fuel Cells, Bockeris JOM, Sriniwasan S. and Mac grow Hills 1969
- 10. Solar Energy Rai C.D.
- 11. Energy Resources, Simon A.L. 1975
- 12. Direct Energy Conversion, Addison Wesley, 1970, All M and Kottani S.
- 13. Outlines in Chemical Technology Vol I, S.D. Sukla & Pandey G.N.M.

# M.Sc. Part-II (Semester-III)

# **Inorganic Chemistry Practical Course ICHP-V and ICHP-VI**

- 1. Ore Analysis -3
- 2. Alloy Analysis 3
- 3. Preparation of coordination complexes
- 4. Ion exchange study of separation of mixtures and estimations
- 5. Spectrophotometry
- 6. Separation and estimation of ions using ion exchange chromatography
- 7. Nephelometry
- 8. Potentiometry
- 9. Conductometry
- 10. Thermal analysis
- 11. Magnetic properties of transition metal complexes
- 12. Spectro Fluorimetry

# 13. Solvent extraction

- 14. Nuclear chemistry
- 15. Soil Analysis
- 16. Data analysis

(Any other experiments may be added when required)

# M.Sc. Part-II (Sem- IV) Inorganic Chemistry

# Paper No. –XIII, ICH 4.1: Instrumental Techniques

# **Unit I: X-ray Diffraction Techniques**

X-ray Sources (X-ray tube and synchrotron sources with their principle of working characteristics of emission spectrum), Bragg's law of diffraction, methods of diffraction (powder and single crystal), Powder diffraction: instrumentation, use of standards, characteristics of powder XRD pattern, significance of peak intensities, systematic absences of reflections, indexing of powder XRD pattern, determination of lattice parameters and solving cubic crystal structure using powder XRD data, qualitative (identification of the phases) and quantitative analysis (phase quantification), crystallite size determination, determination of relative % crystallinity. Single crystal diffraction: Advantages of single crystal diffraction over powder diffraction, introduction to Laue, rotation photograph and oscillation methods. Introduction to crystallographic database and file formats (raw data files, cif and pdf), Open source computer based crystal structure building and visualization tools.

#### **Unit II: Mossbauer Spectroscopy**

Principle of Mossbauer spectroscopy, Recoiless absorption and emission of gamma-rays, Doppler shift, Instrumentation, Isomer shift and its factors affecting, Quadruple splitting, Temperature Dependence of MB parameters, Zeeman Splitting (Six fingered MB lines), MB spectra of iron and tin compounds, Applications, Numericals

# **Unit III: Electron Spin Resonance Spectroscopy**

Principle of ESR Spectroscopy, Presentation of spectrum, Hyperfine splitting in some proton systems, Rules for evaluating ESR lines (Naphthalene anion radical, Pyrazine anion radical, Isomers of Xylene anion radicals, VO<sup>2+</sup>, Quinoline radical, Isoquinoline radical, Quinoxaline radical, Anthracene radical, Phenanthracne radical, Pyrene radical, Alkyl halide radicals, Quinone & Isoquinone anion radicals, nitrogen/deuterium containing radicals), Superhyperfine splitting, Instrumentation,'g' value and factors affecting it, Zero field splitting, Karmers's degeneracy, Applications, Numericals.

# Unit-IV: Introduction to Advanced Instrumental Tools for Analysis of Inorganic materials: 15 Hrs.

Time resolved studies of chemical reactions such as material synthesis (solid state, hydrothermal, sol/gel, thin film growth etc., cathode/anode materials in lithium ion batteries during charge/discharge cycles, in situ X-ray diffraction methods for thermal expansion/contraction studies, structural studies as a function of temperature and pressure (XRD methods), Temperature programmed techniques (temperature programmed desorption/oxidation/reduction: TPD/TPR), methods of determination of surface acidity and basicity of solid catalysts, Computer softwares for plotting and analysis of the XRD data, Structure drawing softwares (VESTA)

#### 15 Hrs.

# 15 Hrs.

15 Hrs.

### **Reference Books**

- 1. Powder Diffraction Theory and Practice, Edited by R E Dinnebier and S J L Billinge, RSC publishing, 2008.
- 2. Catalysis, Principles and Applications, Editors: B. Viswanathan, S. Sivasanker, A.V. Ramswamy, Narosa Publishing House
- 3. VESTA 3 for three-dimensional visualization of crystal, volumetric and morphology data, K. Momma and F. Izumi (2011), J. Appl. Crystallogr., 44, 1272-1276.
- 4. Elements of X-ray Diffraction, B.D. Cullity, Second Edition, Addison Wesley, 1978. Neutron Scattering in Chemistry, Baun, G.E. Butleworth, London, 1971.
- 5. Mossbaur Spectroscopy, Greenwood N.N., Gibbs T.C., Chapmann Hall, 1971.
- 6. Chemical Application of Mossbaur Spectroscopy, Goldanski V.I & Harber R.H., Academic Press 1968.
- 7. Spectroscopy in Inorganic Compounds CNR Rao & Ferraro G.R., Academic Press, 1970.
- 8. Basic Principles of Spectroscopy Cheney R.Mac Grows Hill, 1971.
- 9. Thermal Method, Wendlandt, W.W. John, Wiley, 1986.
- 10. Principles of Instrumental analysis, Skoog, III rd edn., Sounders, 1985.

# Paper No. –XIV, ICH 4.2: Coordination Chemistry-II

# Unit-I Reaction Mechanism of Transition Metal complexes-I

15 Hrs.

Energy profile of reaction. Inert and labile complexes, interpretation of liability and inertness of transition metal complexes on the basis of VBT and CFT. Factors affecting the liability of a complex, transition state or activated complex, substrate, attacking reagents electrophilic and nucleophilic, Nature of central atom. Reactions of metal complexes, ligand substitution reaction, Kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct & indirect evidences in favour of conjugate mechanism, anation reaction.

# Unit-II Reaction Mechanism of Transition Metal complexes-II

15 Hrs.

Substitution reaction in square planer complexes: the trans effect, Theories of Trans effect, uses of trans-effect, cis effect, Electron transfer reactions. Types of electron transfer reactions, conditions of electron transfer, and mechanism of one-electron transfer reactions, outer sphere and inner sphere mechanisms, two electron transfer reactions, complimentary and non-complimentary electron transfer reactions. Marcus Theory, Cross reactions, Inner sphere Reactions, Recimization and isomerisation in transition metal complexes.

### **Unit-III Photochemistry:**

Absorption, excitation, photochemical laws and quantum yield, Electronically excited states and their life-time measurement, Electronically excited states of Metal complexes, type of photochemical reactions, substitutions reactions, rearrangement reactions, redox reaction, Photochemistry of Coordination compounds, LMCT states and MLCT states, Charge transfer spectra, charge transfer excitations, methods for obtaining charge transfer spectra.

## **Unit-IV Applications of Coordination Compounds.**

Metal Complexes in Analytical Chemistry Inorganic Qualitative Analysis, The 'brown ring' test, Complexometric Titrations, Complexes in Colourimetry, Coordination Compounds in Gravimetry, Stabilization of Oxidation States, Complexes in Separation of Metals. Metal Complexes in Medicinal Chemistry:-Complexation in Food Poisoning, Metal Complexes in Therapy. Metal Complexes in Industrial Processes:-Heavy Metals-protein Complexes in the Rasching Process, The Ziegler-Natta Catalyst, Metal complexes in alkene conversions, Complexes and Electroplating, Complexes in Metallurgy. Copper Metal dissolves in Aqueous Potassium Cyanide, Complexes in water softening. Metal complexes in Agriculture.

# **Reference Books:**

- 1. R. Gopalan and V. Ramlingam: Concise Coordination Chemistry.
- 2. J. E. Huheey, Ellen A. Keiter and Okhil K. Medhi: Inorganic Chemistry: Principle of Structure and Reactivity.
- 3. K. F. Purcell, J. C. Kotz: An Introduction to Inorganic Chemistry.
- 4. F. Basolo and R. Pearsons: Mechanism of Inorganic Reactions: A Study of Metal Complexes in Solution.
- 5. Obe, M. L. Inorganic reaction mechanism, Nelson, London, 1972.
- 6. Taube, electron transfer reactions of metal complex ions in solution. Academic Press, 1970.
- 7. E. S. Gould, Inorganic Chemistry.
- 8. V. Balzani and V. Cavassiti, Photochemistry of coordination compounds, AP, London, 1970.
- 9. K. Burger, Coordination Chemistry Experimental methods, Butterworths.
- 10. K. K. Rastogi and Mukharjee, Fundamentals of photochemistry, Wiley eastern.
- 11. J. G. Calverts and J. N. Pits, Photochemicals of Photochemistry, John Wiley.
- 12. Wells, Introduction to Photochemistry.
- 13. K. M. Macky, R. A. Macky, Modern Inorganic Chemistry, 4<sup>th</sup> edn., Blackie, London-1989.
- 14. B. R. Puri, L. R. Sharma, K. C. Kalia, Principles of Inorganic Chemistry, Vallabh Publications, Delhi,2005.

# Paper No. -XV, ICH 4.3: Chemistry of Inorganic Materials

### **Unit-I: Solid State Materials**

A) Bonding incrystals, Crystal systems and Bravais Lattice, Lattice planes and their designation.Metallic Crystal structures:Face-centered cubic (fcc), body-centered cubic (bcc), hexagonal close-packed (hcp) structure.Radius ratio rule (2, 3,4,6,8 co-ordinate structures), octahedral and tetrahedral voids.Isomorphism and polymorphism, Numericals.

# 15 Hrs.

15 Hrs.

# 15 Hrs.

# **B)** Simple type structures:

AB type: NaCl, CsCl, Zincsulphide (sphalerite or cubic and hexagonal),  $AB_2$  type: Fluorite (CaF<sub>2</sub>), TiO<sub>2</sub>(Rutile), CdCl<sub>2</sub>, CdI<sub>2</sub> structures,  $AB_3$  type: ReO<sub>3</sub>, BiI<sub>3</sub>,  $A_2B_3$  type: Corundum Al<sub>2</sub>O<sub>3</sub>,  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>, Mn<sub>2</sub>O<sub>3</sub>.,  $ABO_3$ type: Perovskite Structures (Barium titanate, lead titanate, CaTiO<sub>3</sub>, FeTiO<sub>3</sub>),  $AB_2O_4$  type- Spinel structure, Normal & Inverse, Factors causing distortion in spinel,  $A_2B_2O_7$  type: Pyrochlores (La<sub>2</sub>Sn<sub>2</sub>O<sub>7</sub>).

#### **Unit-II: Imperfections in Materials**

15 Hrs.

Perfect &Imperfect crystals, point defects, Interstitial, Schottky defect, Frenkel defect, line defect & other entities, thermodynamics of Schottky& Frankel defects.

Dissociation, theory of dislocation, plane defects-Lineage boundary, grain boundary, stacking fault, 3D defects, Defects & their concentrations, ionic conductivity in solids, Non stoichiometric compounds.

Electronic properties of Non-stoichiometric oxides, solid electrolytes, pyknometric& electrical conductivity methods of study of defects, photoradiation effects on solid nature and properties, photography, colour centers, order-disorder changes, defects, imperfection equilibrium, atom movements, and defect interactions.

# Unit III :Synthesis and Characterization of Nanomaterials 15 Hrs

General Introduction to Nanomaterials, Nanoscience and nanotechnology, History.

**Chemical Methods**: Metal nanoparticles: Reduction method, Semiconducting or composite nanomaterials: Hydrothermal and Solvothermal method, Sol-gel, Arrested Precipitation, and other methods include) Langmuir-Blodgett, Micelles-Microemulsions.

**Characterization Tools:** Electron Microscopy (TEM & SEM), Probe Microscopy (STM & AFM), Diffraction Technique (XRD), UV-Visible-NIR spectroscopy, BET.

# Unit IV : Properties and Applications of Nanomaterials 15 Hrs.

**Properties of Nanomaterials:** Optical, Magnetic, Electrical, Mechanical, Structural properties **Illustrative Nanomaterials:** Carbon nanostructures (CNTs, Graphene and its derivatives, fullerenes, Metal oxides (TiO<sub>2</sub> and ZnO)& itscomposites, Quantum dots, Core-Shell nanoparticles, Different morphological nanomaterials.

**Applications in the various fields:** Electronic devices, Energy generation and storage, Automobiles, Sports and toys, Textile Industries, Cosmetics Products, Domestic appliances, Sensors, Biotechnology and medical field, Space and Defense, Catalysis, Environment.

#### **Reference Books**

- 1. New Directions in Solid State Chemistry (Second Eds.), C.N.R.Rao and G. Gopalkrishnan, Cambridge Oxford Press.
- 2. A basic course in crystallography, JAK Tareen, TRN Kutty, Universities press.
- 3. Essentials of crystallography, M.A. Wahab, Narosa Publications.
- 4. Synthesis of Inorgnic Materials: Ulrich Schubert, Nicola Hüsing.
- 5. Solid State Chemistry: Lasley E. Smart, Elaine A. Moore.
- 6. Introduction to Solid State Physics: Charles Kittel.

- 7. Solid State Chemistry: A. H. Hanny
- 8. Wilcox : Preparation and Properties of Solid State Materials: Vol I & II, Dekker
- 9. Hagenmuller, Preparative Methods in Solis State Chemistry
- 10. Lohn Wulff, The Structure and Properties of Materials Vol. IV, Electronic Properties (Wily Eastern)
- 11. ,Chemistry of Imprefect Crystals (Holland) E.A. Kroger
- 12. Solid State Chemistry A. R. West,
- 13. Principles of the Solid State Chemistry, Wiley Eastern. H. V. Keer:

# Paper No. –XVI(A), ICH 4.4(A) : Energy and Environmental Chemistry

# **Unit I: Energy Conversion Devices**

Fuel Cells: Working of Fuel Cells, Types of fuel cells, Current capabilities/uses, Fuel cell stacks and systems, Hydrogen as a fuel,

Production of hydrogen: Electrolysis, Thermochemical Processes, Steam Reformer Processes, Water Gas Processes, Bosch Process, Biosynthesis and Photochemical Processes, Coal Gasification, Steam Iron Process, Partial Oxidation Processes. Storage, Transport, and Handling of Hydrogen

# **UNIT II: Energy Storage Devices Batteries**

Li-ion batteries: Principle of operation, Battery components and design, Electrode materials (LiCoO<sub>2</sub>, LiNiO<sub>2</sub>, LiNi<sub>1/3</sub>Mn<sub>1/3</sub>Co<sub>1/3</sub>O<sub>2</sub>, LiMn<sub>2</sub>O<sub>4</sub>, LiFePO<sub>4</sub>, graphitic carbon) their synthesis and characterization, Theoretical capacity, Energy density, power density, cycle life,Electrode and battery fabrication, Battery modules and packs, Li-polymer batteries and applications, Electrolytes for Li-ion batteries, All solid state batteries.Future developments and beyond lithium batteries: Li-S battery, Li-Air battery, Advanced lead-acid batteries, Sodium-battery, Magnesium battery, Aluminum battery, Silicon battery, Battery Recycling Technologies.

# **UNIT III:**

# A) Waste Treatment

Electronic waste recycling programs, E-waste - non-recycling impacts, Materials Used in Manufacturing Electrical and Electronic Products,

Solid Waste Management: Gas to Energy projects, Incandescent vs. compact florescent light bulbs, Value-added Material Recovery, Cost effective treatment of refractory organics,

# **B)** Air and Water Pollution control

Control of NOxSOx and particulate pollution, Sewage and industrial waste water treatment, water softening, municipal water purification

**UNIT-IV:** 

7 Hrs.

8 Hrs.

# 15 Hrs.

15 Hrs.

#### A) Monitoring, sampling and Analysis of Air and water pollutants 8 Hrs.

Methods of monitoring and sampling of gaseous, liquid and solid pollutants, analysis of CO, CO<sub>2</sub>, NO<sub>2</sub>, SO<sub>2</sub>, H<sub>2</sub>S, analysis of toxic heavy metals, Cd, Cr, Hg, As, Pb, analysis of anions  $SO_4^{2^-}$ ,  $PO_4^{3^-}$ ,  $NO_3^{-}$ , estimation of COD and BOD

#### **B)** Techniques in Environmental Analysis

7 Hrs.

ND-IR Spectroscopy, FTIR, AAS, ICP-AES, GC, GC-MS, HPLC, Anodic stripping voltammetry with case studies

# **Reference Books:**

- 1) Lithium ion Batteries: Basics and Applications, R. Korthauer, Springer
- Lithium ion Batteries: Fundamentals and applications, Yuping Wu, CRC Press, Taylor & Francis group
- Lithium ion batteries: Materials, Technology and new applications, K. Ozawa, Wiley
- 30 Years of Lithium-Ion Batteries, Advanced Materials, M. Li et al., Vol 30, issue 33, 2018,1800561
- 5) Fuel Cell Fundamentals, R. O'Hayre, et al., John Wiley & Sons, 2016
- George Techobanoglous et al, "Integrated Solid Waste Management" McGraw Hill, 1993.
- 7) Environmental Chemistry, H. Kaur, PragatiPrakashan, 10<sup>th</sup> edition 2016.
- 8) Environmental Pollution, A. K. De
- 9) Environmental Pollution Analysis, S. M. Khopkar
- 10) Compendium of R&D Projects, Waste Management Technologies (WMT)
   Programme, Technology Development and Transfer Division, Department of
   Science and Technology, New-Delhi 2018-2019.
- Environmental Waste Management, Ed. Ram Chandra, CRC Press 2015, 1<sup>st</sup> Edition
- Electronic Waste Management, RSC Publishers, Editors: R E Hester, R M Harrison, 2009

# Paper No. –XVI(B), ICH 4.4(B): Radiation Chemistry

# **UNIT-I: A] Isotopes**

Difference between Isotopes and Isobars, isotope separation, thermodynamic and kinetic isotope effects, isotope exchange reaction kinetics, determination of exchange rate constant, production and applications of radio isotopes.

# **B**] Biological effects of Radiation

Introduction, genetic and somatic effect on human being, effect of radiation on plants and aquatic Environment.

# **UNIT-II: Radiochemical Separation**

The need of radiochemical separation techniques, carrier techniques, isotope and nonisotopic carriers, coprecipitation and adsorption, ion exchange, solvent extraction, electrolytes behavior of carrier free tracer radionuclide.

# **UNIT-III: Principle of tracer chemistry**

Introduction to tracers, application of tracers in physiochemical studies, diffusion studies, isotopic and exchange reactions, tracer in the study of the mechanism of the inorganic chemical reaction, atom transfer and electron transfer mechanisms. Heterogeneous catalysis and surface area measurements, radio carbon dating, tracer studies with tritium, application in metallurgy and preservation of food, geochemical application and hot atom chemistry.

# **UNIT-IV: Radiation detection and measurements.**

Ionization current measurements, multiplicative ion collector, methods not based on ion collection, auxiliary Instrumentation and health physical instruments and counting statistics. Working of Scintillation and Geiger Muller Counter.

# **Reference Books**

- 1. Friedlander, Kennedy and Miller, Nuclear and radio Chemistry, ohm Wiley.
- 2. B.G. Harvey, Nuclear Chemistry.
- 3. Haissinsky, Translated by D.G, Tuck, Nuclear physics and Chemistry.
- 4. Mark lefort, Nuclear Chemistry, D.V. Nostrand.
- 5. An N.Nesmeyanov, Radiochemistry, Mir.
- 6. Jacobs, et al, Basic Principles of nuclear science and reactors, V.Nost, EW AP.
- 7. N. Jay, Nuclear power, today tomorrow, ELBS.
- 8. Kenneth, Nuclear power, today and tomorrow, ELBS.
- 9. Essentials of Nuclear Chemistry, J. Arnikar, John Wiley.
- 10. D.C. Dayal, nuclear physics.

# 8 Hrs

# 15 Hrs.

# 15 Hrs.

15 Hrs.

# M.Sc. Part-II (Semester-IV)

# Inorganic Chemistry Practical Course ICHP-VII and ICHP-VIII

# Practical courses includes Submission of project work :

# (A) Practicals

- 1. Ore Analysis -3
- 2. Preparation of coordination compounds (Three) and preparations of mixed metal oxides(two)
- 3. Ion Exchange chromatography; separation of multicomponent mixtures
- 4. Solvent extraction
- 5. Spectrophotometry
- 6.  $P^{H}$  Metry
- 7. Conductometry
- 8. Polarography
- 9. Electrogravimetry
- 10. Nuclear and radiochemistry

# **B)** Interpretation exercises

- 1. X-ray powder diffraction analysis of cubic compound
  - a. Determination of lattice constants and geometry
  - b. Partical Size
  - c. Density
- Interpretation of Mossbaur spectrum with reference to determination of a) isomer shift
   b) quadruple splitting c) Internal magnetic field d) general comment
- 3. Interpretation of IR spectrum with reference to stretching vibration 0-2 C=N, C=O, N-, M-O.
- 4. Interpretation of NMR spectrum with reference to calculation of chemical shifts and general comments.
- 5. Interpretation of absorption spectra for
  - a. Verification of position of ligands in spectrochemical series
  - b. Determination of geometry (Octahedral, Square planar, tetrahedral) of a given compound.
  - c. Calculation of spectral splitting parameters.
- 6. Interpretation of polar gram for determination of half wave potentials and unknown concentration.
- 7. Calculation of band gap of semiconductors with the help of plots of log Vs.10  $\frac{3}{4}$ .
- In all 20 experiments with at least five experiments in each course should be completed. Addition of other experiments in place of existing one may be allowed. A variety of small projects designed by teacher based on the interest of students and capabilities should be worked out. (**Project** work or the review report (50 Marks) will be examined by internal and external examiners.

# Study tour is compulsory for M.Sc. Part- II Students to visit Chemical Industries in India.

# M.Sc. Part-II, (Sem-III and IV) Organic Chemistry <u>SEMESTER III</u>

Paper No IX, OCH 3.1	: Organic Reaction Mechanism
Paper No X, OCH 3.2	: Advanced Spectroscopic methods
Paper No. –XI, OCH 3.3	: Advanced Synthetic methods
Paper No XII(A), OCH 3.4(A)	: Drugs and Heterocycles
Paper No. XII(B), OCH 3.4(B)	: Polymer Chemistry
Practical Course	: OCHP-V and OCHP-VI

# SEMESTER IV

Paper No. – XIII, OCH 4.1	: Theoretical Organic Chemistry
Paper No. XIV, OCH 4.2	: Stereochemistry
Paper No. – XV, OCH 4.3	: Chemistry of Natural Products
<b>ELECTIVE PAPERS</b> Paper No XVI(A), OCH 4.4(A)	: Applied Organic Chemistry
Paper NoXVI(B), OCH 4.4(B)	: Bioorganic Chemistry
Practical Course	: OCHP-VII and OCHP-VIII

#### M.Sc. Part-II (Sem- III) Organic Chemistry

#### Paper No.- IX, OCH 3.1: ORGANIC REACTION MECHANISM

# UNIT-I: Methods of determining reaction mechanism

**Kinetic Methods:** Order and Molecularity, Methods of following reaction rates, Types of reactions: 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> order reactions; Reversible, Consecutive and Parallel reactions. Energy of Activation, Entropy of Activation, Effect of Ionic strength, Solvent effect and Kinetic isotopic effect

**Non-Kinetic Methods:** Identification of reaction products, Testing of the possible intermediates, trapping of the intermediates, isotopic labeling, Reaction catalysis, Cross-over experiments, Stereochemical studies and Use of physical properties. **Hammett and Taft equations.** 

# **UNIT—II: Pericyclic reactions**

Molecular orbital symmetry, Frontier orbital of ethylene, 1,3- butadiene, 1,3,5-hexatriene and allyl system, classification of peri cyclic reaction, Wood-ward Hoffman correlation diagrams, FMO and PMO approach, electrocyclic reactions, conrotatory and disrotatary motions, 4n, 4n+2 and allyl systems, cycloaddition, and supra and antara facial additions, 4n and 4n+2 systems, 2+2 additions of ketenes, 1,3-dipolar cycloaddition and chelotropic reactions, sigmatropic rearrangement, supra and antarafacial shifts of H, Sigmatropic shifts involving carbon moieties, (3,3) and (5,5) sigmatropic rearrangement and Claisen and Cope and Aza Cope rearrangement, Ene reaction.

# UNIT — III:

**A) Study of reactive intermediates:** Synthesis and applications of nitrogen, sulphur and phosphorous ylides. (7)

B) Study of following reactions: Alkyne metathesis reaction, Weinreb ketone synthesis, Petasis reaction, Henry reaction, Corey Kim oxidation. Reactions of carboxylic acids and esters.
 (8)

#### **UNIT-IV: Free radical reactions**

Types of free radical reactions, detection by ESR, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in attacking radicals. The effect of solvent on reactivity. Allylic hydrogenation (NBS), oxidation of aldehydes to carboxylic acids, auto oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salt, Sandmeyers reaction. Hunsdiecker reaction.

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# **RECOMMENDED BOOKS:**

- 1. A guide book to mechanism in organic chemistry (orient- Longmans)- Peter Sykes
- 2. Organic Reaction Mechanism (Benjumin)- R. Breslow
- 3. Mechanism and structure in Organic Chemistry (Holt Reinhartwinston)- B. S. Gould
- 4. Organic chemistry (McGraw Hill)- Hendrikson, cram and Hammond
- 5. Basic principles of organic chemistry (Benjamin) J. D. Roberts and M. C. Caeserio.
- 6. Reactive intermediates in organic chemistry, (J. Wiley) N. S. Issacs.
- 7. Organic reaction mechanism (McGraw Hill ) R. K. Bansal
- 8. Fundamentals of photochemistry K. K. Rohtagi- Mukherji Wiley- Eastern
- 9. Essentials of molecular photochemistry, A. Gilbert and J. Baggott. Blackwell Scientific Publication.
- 10. Molecular photochemistry, N.J. Urro, W. A. Benjamin
- 11. Introductory photochemistry. Cox and T. Camp McGraw -Hill
- 12. Photochemistry R.P. Kundall and A. Gilbert. Thomson Nelson.
- 13. Strategic applications of named reactions in organic synthesis by Laszlo Kurti and Barbara Czako.
- 14. Organic photochemistry J. Coxon and B. Hallon Cambridge University press.

### Paper No. -X, OCH 3.2: ADVANCED SPECTROSCOPIC METHODS

# UNIT-I:

A) Ultraviolet Spectroscopy: Woodward- Fisher rules for conjugated dienes and carbonyl compounds; Calculation of  $\lambda$  max. Ultraviolet spectra of aromatic and heterocyclic compounds, Steric effect in biphenyls. (05)

**B) IR Spectroscopy:** Characteristic vibrational frequencies of alkanes; alkenes; alkynes; aromatic compounds; alcohols; ethers; phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds [ketones; aldehydes; esters; amides; acids; anhydrides; lactones; lactams and conjugated carbonyl compounds] Effect of hydrogen bonding and solvent effect on vibrational frequencies; overtones; combination bands and Fermi resonance. FT-IR of gaseous; solids and polymeric materials. (10)

# **UNIT-II: NMR Spectroscopy**

General introduction and definition; chemical shift; spin –spin interaction; shielding mechanism of measurement; chemical shift values and correlation for protons bonded to carbons [aliphatic; olefinic; aldehydic and aromatic] and other nuclei [alcohols; phenols; enols; acids; ammines; amides and mercaptons]; chemical exchange; effect of deuteration; complex spin-spin interaction between two; three; four; and five nuclei [first order spectra]; virtual coupling.

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Stereochemistry; hindered rotation; Karplus curve variation of coupling constant with dihedral angle. Simplification Simplification of complex spectra; nuclear magnetic double resonance; shift reagent; solvent effect. Fourier transform technique, nuclear overhauser effect [NOE] Resonance of other nuclei – F; P.

# **UNIT-III: Mass Spectrometry**

Introduction, ion production- EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement, nitrogen rule. High-resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

# UNIT – IV:

A) Carbon-13 NMR Spectroscopy: General considerations; chemical shift [aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl compounds]; problems associated with <sup>13</sup>C, FT-NMR, proton decoupled off resonance. (07)

# B) Structural problems based on combined spectroscopic techniques (including reaction sequences) (8)

#### **RECOMMENDED BOOKS:**

- 1. V.M. Parikh, Application spectroscopy of organic molecules. (Mehta)
- 2. D.W. Williams and Flemming, Spectroscopic methods of organic compound.
- 3. Silverstein and Basslar, Spectroscopic identification of organic compounds V.M. Parikh ORPTION SPECTROSCIPY OF ORGANIC MOLECULES (J. Wiley)
- 4. P.S. Kalsi Spectroscope of organic compounds (New age publisher)
- 5. J.R. Dyer. Application of absorption spectroscopy of organic compounds.
- 6. Jackman and Sterneil, Application of NMR spectroscopy
- 7. Nuclear magnetic resonance. J.D. Roberts (J. Wiley)
- 8. Theory and application of U.V. Jafee and Orchin.
- 9. Mass spectroscopy K. Benjamin.
- 10. The mass spectra of organic molecules. Beynon J H.
- 11. Interpretation of carbon 13 NMR Wehli F.W, Marchand A. P. (J. Wiley)
- 12. Organic Spectroscopy W. Kemp, ELBS
- 13. Instrumental methods of analysis CBS. Willard Merritt and Dean.
- 14. Mass Spectroscopy. Das and Jame
- Organic structural spectroscopy : J. B. Lambert, S. Gronert, H. F. Shurvell, D. Lightneli, R. G. Cooks (Prentice Hall 2<sup>nd</sup> edition)

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# Paper No. – XI, OCH 3.3 : ADVANCED SYNTHETIC METHODS

# **UNIT-I: Disconnection approach**

An introduction to Synthons and synthetic equivalents, disconnection approach, functional group interconversions. One group C-X and two group disconnections in1, 2; 1, 3 - 1, 4 & 1, 5-difunctional compounds, Retro - synthesis of alkene, acetylenes and aliphatic nitro alcohols and carbonyl compounds, amines. Importance of the Order of events in organic synthesis, Chemoselectivity, Regioselectivity. Protecting groups, Diels-Alder reaction, Michael addition and Robinson annulation. Retro- synthesis of aromatic heterocycles and 3, 4, 5 and 6 membered carbocyclic and heterocyclic rings. Reversal of polarity (Umpolung).

# UNIT–II: Applications of the following reagents in organic synthesis. (15)

Lithium diisopropylamide(LDA) Dicyclohexyl carbodiimide(DCC), lead tetra acetate, PPA, Diazomethane, ozone, phase transfer catalyst, Woodward-Prevost hydroxylation, Barton and Shapiro reaction, Hoffmann – Loffler-Fretag, Peterson synthesis, Selenium dioxide, Dess-Martin periodinane, periodic acid and iodoisobenzyldiacetate, Olefin metathesis using Grub's catalysts.

UNIT-III:	(15)
A) Applications of following metal in organic synthesis	
Ti, Ce, Tl and Si	(07)
<b>B)</b> Synthesis and applications of following ligands in organic synthesis. Phosphines, N-heterocyclic carbenes, Oxazoline ligands	(08)

# UNIT–IV: Application of the following in synthesis (15)

Synthesis and applications of Merrifield resin, Electro-organic synthesis, Enzyme catalyzed reaction in synthesis, Solvent free synthesis, Multicomponent reactions, Microwave and Ultrasound techniques and their applications.

# **RECOMMENDED BOOKS:**

- 1. Designing of organic synthesis. S. Warren
- 2. Organic synthesis J. Fuhrhop & G. Penzlin. (2nd ed.)
- 3. Some modern methods of organic synthesis.Carruthres:
- 4. Modern synthetic reaction. H. O. House
- 5. Reagent in organic synthesis. Fieser & Fieser
- 6. Principle of organic synthesis. R. O. C. Norman
- 7. Advanced organic Chemistry. Carey & Sundharg
- 8. Organic synthesis. P. E. Realand:

- 9. Comprehensive organic Chemistry. Bartan and Ollis :
- 10. Organic reactions. R. Admas:
- 11. Advances in organometallic Chemistry. Stone & West:
- 12. Transition metal intermediate in organic synthesis. C. W. Bird:
- 13. Organometallic in organic synthesis. Swan & black :
- 14. Synthesis of prostaglandins. A. Mitra :
- 15. Total synthesis of natural products. John Apsimon:
- 16. Phosphorus ligands in homogeneous catalysis: Design and synthesis by Paul C. J. Kamer.
- Phosphorus ligands effect in homogeneous catalysis and rational catalyst design by Jason A. Gillespie and Erik Zuidema. Polymers as aid in organic synthesis. M. K. Mathur, C. K. Narang & R. E. Williams:
- 18. Polymer supported reaction in organic synthesis. P. Hodge & D. C. Sherrington:
- 19. Enzyme catalysed reactions.C. J. Gray:
- 20. Electroorganic Chemistry. T. Shona:
- 21. Phase transfer catalyst in organic synthesis. Weber & Gokel :

# Paper No.- XII (A), OCH 3.4(A) : DRUG AND HETEROCYCLES

# Part- A: Drugs

# UNIT-I:

# A) Drug design

Procedures followed in drug design, **factors affecting development of new drugs**, concepts of prodrugs and soft drugs, **Isosterism**, **bioisosterism**, Theories of drug activity, Quantitative structure activity relationship, QSAR theory, Concepts of drug receptors. (10)

# **B) Study of Antibiotics**

Classification of antibiotics, Preparation of semi synthetic penicillin, Penicillin G, Penicillin V, conversion of penicillin into cephalosporin. (05)

# UNIT-II: Study of the Following types of drugs

- a) Antimalerials: Trimethoprim, Amodiaquine
- b) Analgesic & Antipyretics: Meperidine, Aminopyrine, Diflunisal
- c) Anti- inflammatory: Oxyphenylbutazone, Indomethacin
- d) Antitubercular & antileprotic: Dapsone, Pyrazinamide, Ethionamide
- e) Anaesthetics: Lidocaine, Thiopental

# f) Antihistamines: Cyproheptadine, Cetirizine

g) Psychoactive drugs: Ethiosuximide, Glutethimide

(15)

h) Antiinfective drugs: Grisefulvin, norfloxacin

h) Anti AIDS: General study

i) Cardiovascular: Synthesis of warfarim, Clofibrate, quinidine, methyldopa, atenolol

**j)** Anti-neoplastic drugs: Cancer chemotherapy, Synthesis of mechloraethamine, cyclophosphamide, Mephalan, uracils, mustards. Recent development in cancer chemotherapy. Hormones and natural products.

# **Part-B: HETEROCYCLES**

(15)

(15)

#### UNIT-III:

A) Small ring Heterocycles: Three membered and four membered Heterocycles- synthesis and reactions of aziridines, oxiranes, thiranes, azetidines (05)
 B) Benzofused five membered Heterocycles : Synthesis and reactions of benzopyrroles, benzofurans and benzothiophenes (05)
 C) Six membered Heterocycles with one heteroatom: Synthesis and reactions of pyrilium salts and pyrones, coumarins, chromones. (05)

## UNIT – IV:

A) Six membered Heterocycles with two and more Heteroatoms: Synthesis and reactions of diazines & triazines (08)
 B) Benzofused heterocycles with two hetero atom: Synthesis and reactions of benzimidazole, benzthiazole and benzoxazole (07)

# **RECOMMENDED BOOKS:**

1. Medicinal Chemistry.Burger:

- 2. Medicinal Chemistry A. Kar. (Wiley East)
- 3. Principals of medicinal chemistry.W. O. Foye:
- 4. Text book of organic medical and pharmaceutical chemistry. Wilson, Gisvold & Dorque:
- 5. Pharmaceutical manufacturing encyclopedia.
- 6. D. Sriram, P. Yogeeswari: Medicinal Chemistry
- 7. An introduction to chemistry of heterocyclic compounds. R. M. Acheson : (Interscience).
- 8. Heterocyclic chemistry. Joule & Smith: (Van Nostrand).
- 9. Heterocyclic chemistry. R. K. Bansal: (Wiley E).
- 10. Principals of modern heterocyclic chemistry.L. A. Paquitte:
- 11. The structure and reactions of heterocyclic compounds.M. H. Palamer:
- 12. Advances in Heterocyclic chemistry. A. R. Katritzky: (A.P.).
- 13. Organic chemistry (Vol. 1& 2) Finar.
- 14. Outline of Biochemistry. Cohn & Stumpt
- 15. Introduction to the chemistry of enzyme action. Williams:
- 16. The Organic Chemistry of Drug design and Drug action. R. B. Silverman Academic press.
- 17. Strategies for Organic Drug synthesis and Design. D. Lednicer, J. Willey.
- 18. Heterocyclic Chemistry. Vol-1-3, R. R. Gupta, M. Kumar and V. Gupta, Springer Veriag.
- 19. The Chemistry of Heterocycles. T. Eicher and S. Hauptmann, Thieme

- 20. Heterocyclic Chemistry. J. A. Joule, K. Mills and G. F. Smith, Chapman and Hall
- 21. Heterocyclic Chemistry. T. L. Gilchrist, Longman Scientific Technical
- 22. Contemporary Heterocyclic Chemistry. G. R. Nikome and W. W. Poudler, Willey
- 23. An Introduction to Heterocyclic Compounds, R. M. Acheson, J. Willey
- 24. Comprehensive Heterocyclic Chemistry. A. R. Katritzky and C. W. Rees

# PAPER NO. - XII (B), OCH 3.4(B): POLYMER CHEMISTRY (OPTIONAL PAPER FOR SEM-III)

#### **UNIT-I:**

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**Terminology and basic concepts of Polymers**: Monomers, Functionality, repeat units, degree of polymerization. General structure and naming of polymers. Average molecular weight and average chain dimension concept. Expressions for average molecular weighs. Molecular weight distribution and Polydispersity. Classification based on various considerations-source, preparation methods, thermal behavior, chain structure etc.

Types –Homopolymers and copolymers; linear, branched and network polymers.

**Techniques of polymerization**: Techniques of preparation of addition and condensation polymers.

**Kinetics of Polymerization**: Kinetics and mechanism of addition and condensation polymerization. Kinetics of copolymerization-reactivity ratio and copolymer equation. Free radical chain polymerization- Cationic polymerization – Anionic polymerization – Poly condensation. Glass transition temperature: Glassy solids and Glass transition – associated properties – Factors influencing glass transition temperature – molecular weight – Plasticisers – melting point – importance of glass transition temperature.

# **UNIT-II:**

**Crystalline Nature:** Crystalline soils and their behaviour towards X-rays – Polymers and X- ray diffraction – Degree of crystallinity – crystallites –factors affecting crystallinity, Helix structures.

**Copolyemerization:** Free radical copolymerization – Ionic copolymerization – Copolycondensation – Individual monomers: Polyethylene, polypropylene, polystyrene, poly acrylonitrile, polymethyl methacrylate, polyesters, polycarbonates, polyamides, polyurethanes, polyvinyl acetate, polyvinyl chloride, poly isoprene's, silicone polymers.

# UNIT-III:

**Polymer degradation:** Types of degradation, thermal and mechanical – photo degradation – oxidative and hydrolytic degradation. Polymer reactions – Hydrolysis, acidolysis, aminolysis, hydrogenation, addition and substitution reactions – cyclisation, cross-linking reactions – Graft and Block copolymers.

Experimental methods: Polymer synthesis, isolation and purification of polymers -

Fractional - Molecular weight determination – Molecular weight distribution curve – determination of glass transition temperature. Elastomeric materials – Fibre forming materials – Plastic material Rheology of polymeric materials – compounding and processing techniques.

# UNIT-IV:

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**Stereochemistry of polymers**: Geometric and optical isomerism in polymers. Structure, properties and preparation of stereoregular polymers.

Determination of molecular weight: Osmometry and viscometry.

**Thermal Characterization**: Glass Transition and melting-correlation with structure-Factors affecting Tg and Tm. Techniques of thermal characterization: DSC, DTA, DTG and TGA techniques.

**Structural features, properties and uses of commercial polymers:** Polyethylene, polystyrene, PVC, polyesters, polyamides, polyurethanes and polycarbonates. Conducting polymers, liquid crystal polymers and biomedical polymers.

# **RECOMMENDED BOOKS:**

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- 1. Contemporary Polymer Chemistry-H.R. Allcock and F.W. Lampe (Prentice Hall).
- 2. Polymer Science and Technology-J.R. Frird (Prentice Hall).
- 3. Polymer Science: V.R. Gowariker, N.V.Viswanathan & T.Sreedhar
- 4. Principles of Polymer Science- P.Bahadur and N.V.Sastry (Narosa Publishers)
- 5. 'Organic Polymer Chemistry', K.J.Saunders, Chapman and Hall, 1976.
- 6. 'Polymer Chemistry An Introduction', Raymond B.Seymour, Marcel Dekker Inc., New York and Based, 1981.
- 7. 'Text Book of Polymer Science', Fred W.Billmeyer, Jr.John-Wiley and Sons, 3rd Edn. 1984.
- 8. 'Fundamentals of Polymer Science and Engineering', Kumar Gupta, Tata Mc Graw Hill, 1981.
- 9. "Polymer Characterization of Processing Technolgy', Stepak, Academic Press, London.
- 10. 'Inorganic Polymers', Stone, Academic Press, New York.
- 11. Polymer Chemistry, B.K.Sharma, Krishna Prakashan Mandir, Meerut.

# M.Sc. Part-II (Semester-III) Organic Chemistry Practical Course OCHP- V and OCHP- VI ative Analysis

# A. Qualitative Analysis

Separation, purification and identification of compounds of ternary mixtures using **semi-microanalysis**, TLC, column chromatography and chemical tests. IR spectra tobe used for functional group identification.

# **B.** Quantitative analysis

# 1. Two step Preparations (Any Five)

- a) Preparation of m-Nitroaniline
- b) Preparation of Benzanilide from benzophenone
- c) Preparation of Phthalimide
- d) Preparation of N-Bromosuccinimide
- e) Preparation of 4-methyl -7-acetoxy coumarin
- f) Preparation of 1, 2, 3, 4- Tetrahydro carbazole
- g) Preparation of p-ethoxy acetanilide
- 2. Colorimetry and pH metry experiments.
- 3. Expt. on Hammett equation
- 4. Structure elucidation by using given spectral data.

# 5. Any other suitable expt. may be added

# **RECOMMONDED BOOKS:**

- 1. Textbook of Practical Organic Chemistry A. I. Vogel.
- 2. Practical Organic Chemistry Mann & Saunders.
- 3. A Handbook of Quantitative & Qualitative Analysis- H. T. Clarke.
- 4. Organic Synthesis Collective Volumes by Blat

# M. Sc. Part -II (Sem - IV) Organic Chemistry

# Paper No.- XIII, OCH 4.1: THEORETICAL ORGANIC CHEMISTRY

# **UNIT-I: Molecular Orbital Theory**

Aromaticity in benzenoids, alternant and non alternant hydrocarbon, Huckels rule, energy level of pi- molecular orbital and concept of aromaticity, calculation of energies of orbitals cyclic and acyclic systems. Determination energies and stabilities of different systems calculation of charge densities PMO theory and reactivity index.

# UNIT – II: Non benzenoid aromatic Compounds (15)

Aromaticity in Non- benzenoids compounds Annulenes and heteroannulenes, fullerenes, azulene, fulvene, tropylium salts, ferrocene, five membered systems. Crown ether complexes, cyclodextrins, cryptands, catenanes and rotaxanes, bonding in fullerenes.

# UNIT – III: Green chemistry

Introduction to the principles of green chemistry – prevention of waste, atom economy, less hazardous chemical syntheses, designing safer chemicals, safer solvents and auxiliaries, design for energy efficiency, reduce derivatives, renewable feedstock, catalysis, design for degradation, real time analysis for pollution prevention, and inherently safer chemistry for accident prevention. Green synthesis, clean routes using supercritical solvents, ionic liquids and water.

# UNIT – IV A) Kinetic and thermodynamic control of reactions

Nitration and Sulphonation of naphthalene, Wittig, Enolization, Friedel-Crafts and Diels Alder reactions.

# B) Non-classical carbocations: Formation, stability and reactivity. (6)

# **RECOMMENDED BOOKS:**

- 1. 1. Lehar and Merchand: Orbital Symmetry.
- 2. R. B. Woodward and Hoffman: Conservation of orbital symmetry.
- 3. P. T. Anastas, J. C. Werner: Green Chemistry: Theory and Practice
- 4. V. K. Ahluwalia: Green chemistry, A textbook
- 5. V. K. Ahluwalia, R. S. Verma: Green Solvents: For Organic Synthesis
- 6. Ginsburg: Nonbenzenoid aromatic compound.
- 7. A. Streitwieser: Molecular orbital theory for organic chemistry.
- 8. E. Cler: The aromatic sextet.
- 9. Lloyd: Carbocyclic non- benzenoid aromatic compounds.
- 10. W. B. Smith: Molecular orbital methods in organic chemistry.
- 11. Grratt; Aromaticity

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# Paper No. - XIV, OCH 4.2: STEREOCHEMISTRY

### UNIT-I:

Conformational analysis and reactivity of acyclic and alicyclic compounds	(15 h)
(A) Conformational analysis of acyclic compounds	(4 h)

The difference between configuration and conformation. Klyne-Prelog terminology for torsion strain, Pitzer strain, van der Waals interactions, hydrogen bonding, and gauche effect. Conformations of 2, 3-dimethylbutane, 1,2-dihaloethanes, ephedrine.

#### (B) Conformational analysis of cyclohexane derivatives (4 h)

Concept of Baeyer ring strain, ring inversion, locking groups. Conformations of (1, 4-di-tbutylcyclohexane, 1, 4-cyclohexanediol, menthol, cyclohexanone.

(C) Effect of conformation on reactivity (mechanism) of acyclic and cyclic systems (7 h) Curtin-Hammett principle. Effect of conformation on the course and rate of reactions in cyclohexane; debromination of 2,3-dibromobutane, semipinacolic deamination of 1,2-diphenyl-1-(pchlorophenyl)-2-amino ethanol, dehydrohalogination of stilbene dihalide and bromo-1,2diphenyl propane, stereochemistry of molecular rearrangements; pyrolytic cis-elimination.

# UNIT- II: Conformational analysis and reactivity of cyclic compounds other than six membered (15 h)

#### (A) Fused rings

Types of fused ring systems; (a) Fused bicycles: cis and trans-decalins, octalins, decalols,(b) Fused polybicycles: perhydroanthracene,

(10 h)

(5 h)

# (B) Bridged rings

Types of bridged ring systems, nomenclature, bridged bicycles: heptanes and octane, stereo chemical restrictions, Bredt's rule.

#### UNIT III: Stereoselective synthesis (15 h)

(A) Stereoselective addition of nucleophiles to carbonyl group: Cram's rule, Felkin Ahn rule, Houk model, Cram's chelate model. Asymmetric synthesis by use of chiral auxiliaries. Nucleophilic addition: use of chiral substrates, auxiliaries, reagents and catalysts (B) Asymmetric Oxidations: Asymmetric epoxidation of allylic alcohols (Sharpless Epoxidation), dihydroxylation of olefins (Sharpless asymmetric dihydroxylation, Upjohn process, Milas hydroxylation).

(C) Asymmetric Diels-Alder Reactions using chiral Lewis acids: Chiral bissulfonamides (Corey's catalyst).

UNIT-IV: Stereochemistry of compounds containing no chiral carbon atoms	(15 h)
(A) Stereochemistry of allens, sprains and biphenyls, assignment of configuration	(4 h)
(B) Configuration of diastereomers: Geometrical isomerism based on physical an	d chemical
methods.	(4 h)

#### (7 h) (C) O.R.D. and C.D.

ORD and CD curves with Cotton effect. Empirical and semi-empirical rules; The octant rule, helicity rule, Lowe's rule, and axial haloketone rule.

# **RECOMMENDED BOOKS:**

1. E.L. Eliel: Stereochemistry of carbon compounds.

- 2. D. Nasipuri : Stereochemistry of organic compounds
- 3. P.S. Kalsi: Stereochemistry, Conformation and Mechanism.
- 4. Eliel, Allinger, Angyal and Morrison: Conformational analysis.
- 5. Hallas: Organic stereochemistry
- 6. Mislow and Benjamin: Introduction to Stereochemistry.
- 7. H. Kagan: Organic stereochemistry.
- 8. Carl Djerassi; Optical Rotatory Dispersion.
- 9. P. Crabbe : Optical Rotatory Dispersion and C.D.

# Paper No. – XV, OCH 4.3: CHEMISTRY OF NATURAL PRODUCTS

#### **UNIT-I:**

A) Introduction of natural products and Terpenoids: Introduction of natural products: Classification and isolation methods. Terpenoids: Structure and synthesis of camphor, carvone, abietic acid, zingiberene,  $\alpha$ -santonin,  $\beta$ -cuparenone. Biogenesis of abietic acid.

#### **UNIT-II:**

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**Alkaloids:** Structure, stereochemistry, synthesis and biosynthesis of the following: Morphine, Reserpine, Papaverine and Lysergic acid. Biogenesis of Coniine.

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#### **UNIT-III:**

Steroids: Occurrence, nomenclature, basic skeleton, Diels hydrocarbon.

**Study of the following:** hormones (Structure and synthesis): Cholesterol, Androsterone, Testosterone, Estrone, Progesterone, Aldosterone and cortisone Bile acid (only synthesis) and biosynthesis of lanosterol.

#### **UNIT-IV:**

A) Prostaglandins: Occurrence, nomenclature, classification, biogenesis and physiological effects, Synthesis of PGE2 and PGF2.
 (05)

B) Lipids: Classification, Role of Lipids, Fatty acids and glycerol derived from oils and fats.(04)

C) Vitamins: Synthesis and structure of biotin, vitamin B1 and B2, Biological functions of Vitamin B<sub>6</sub>, D and E. (06)

#### **RECOMMENDED BOOKS:**

- 1. Apsimon: The total synthesis of natural products.
- 2. Manskey and Holmes: Alkaloids
- 3. A.A. Newmen: Chemistry of Terpenes.
- 4. P. D B. Mayo: The chemistry of natural products.
- 5. Simonson: Terpenes.
- 6. T.W. Goddwin: Aspects of terpenoid chemistry and biochemistry.
- 7. Woguer: Vitamins and Co- enzymes.
- 8. P. W. Bently: Chemistry of Natural products,
- 9. Fieser and Fieser: Steriods
- 10. I. Finar: Organic chemistry Vol. II and I
- 11. J.B. Hendrickson, The molecules of nature.

12. Peter Bernfield: The biogenesis of natural products

13. R.T. Slicken staff A.C. Ghosh and G.C. Wole: Total synthesis of steroids.

- 14. The chemistry of natural products, vol. Nakanishi
- 15. Biochemistry of Lipids, Lipoproteins and membranes by Neele Ridgway and Roger McLeod
- 16. Membranes (New comprehensive biochemistry) by J E Vance and E Vance

17. Schaum's easy outline of biochemistry by Philip W Kuchel.

#### Paper No. - XVI (A), OCH 4.4(A): APPLIED ORGANIC CHEMISTRY

#### **UNIT-I:**

#### A) Agrochemicals

a. Organochlorine pesticides: Introduction, synthesis and mode of action of endrin, aldrin, dieldrin.

b. Herbicides: Synthesis and mode of action of Triazines, triazoles, pyridazinones and Bipyridylium compounds: diquat, paraquat.

f. Juvenile harmone: introduction & structures JHA importance synthesis, IPM	(08)
B) Synthesis and applications of perfumery	
2-Phenylethanol, vanillin and other food flavours, synthetic musk and ionones.	(07)

#### **UNIT- II Unit Processes**

Introduction, Nitration of hydrocarbons, Becamp reduction, halogenations, sulphonation of aromatic compounds.

#### **UNIT-III: Dyes and Intermediates**

Classification and synthesis of important dye intermediates by using nitration, sulphonation, diazotization reactions. Synthesis of Nitro dyes, xanthenes, reactive dyes, Fluorescent brightening agents, thermal sensitive dyes, dispersed dyes and reactive dyes.

#### **UNIT-IV: Polymers**

Mechanism of polymerization. Industrial process for synthesis of polyethylene, acrylonitrile, acrylate and methaacrylate polymer, biomedical polymer, Polymer processing, Plasticizers and anti-oxidants for polymers,

#### **RECOMMENDED BOOKS:**

- 1. Allan: Colour Chemistry
- 2. K. Venkataraman: Chemistry of Synthetic Dyes Vol-1 to 7
- 3. G. R. Chatwal: Synthetic dyes

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- 4. Abrahart: Dyes & their intermediates
- 5. N. N. Melikov: The Chemistry of Pesticides and formulations
- 6. K. H. Buchel: Chemistry of Pesticides.
- 7. R. Clemlyn: Pesticides
- 8. K. H. Buchel: Chemistry of Pesticides
- 9. H9. R. Alcock and F. W. Lambe: Contemporary Polymer Chemistry
- 10. J. 10M. G. Cowie, Blackie: Physics & Chemistry of Polymers
- 12. I. M. Campbell: Introduction to Synthetic Polymers
- 13. A. L. Gupta: Polymer Chemistry
- 14. M. S. Bhatnagar: A textbook of Polymers
- 15. F. W. Billmeyer: Textbook of Polymer Science
- 16. P. H. Groggins: Unit Processes in Organic Synthesis
- 17. B. Biollot& P. V. Wells: Perfumary Technology
- 18. M. Ash & I. Ash: A formulary of Cosmetic Preparations

#### Paper No. - XVI (B), OCH 4.4(B): BIOORGANIC CHEMISTRY

#### (ELECTIVE CBCS PAPER)

#### **UNIT-I:**

#### **A) Cell Structure and Functions**

Structure of prokaryotic and eukaryotic cells, Intracellular organelles and their functions, comparison of plant and animal cells. Overview of metabolic process- catabolism and anabolism. ATP - the biological energy currency. Origin of life- uniqueproperties of carbon, chemical evolution and rise of living system. Introduction to biomolecules, building blocks of biomacromolecules. (10)

#### **B)** Enzymes

Structure activity and reactions, catalyzed determination of active site, inhibition mechanism chemical transformations using enzymes.

#### **UNIT-II: Carbohydrates**

#### (15)

Conformation of monosaccharides, structure and functions of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinositol, amino sugars. Naceylmuramic acid, sialic acid disaccharides and polysaccharides. Structural polysccharides- cellulose and chitin. Storage polysaccharides- starch and glycogen.

#### (5)

Structure and biological functions of glucosaminoglycans or mucopolysaccharides. Carbohydrates of glycoprotines and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid.

Carbohydrate metabolism- Kerb's cycle, glycolysis, glycogenesis and glycogenolysis, pentose phosphate pathway.

#### **UNIT-III: Lipids**

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Fatty acids, essential fatty acids, structures and function of triglycerides, glycerophspholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Lipoproteins-composition and function, role in arthrosclerosis. Properties of lipid aggregates – micelles, bilayers, liposomes and their possible biological functions. Biological member's .Fluid mosaic model of membrane structure. Lipid metabolism -  $\beta$ -oxidation of fatty acids

#### UNIT-IV: a) Amino acids, Peptides and Proteins

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of protein, forces responsible for holding of secondary structures.  $\alpha$ - helix,  $\beta$ -sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein- folding and domain structure. Quaternary structure. Amino acid metabolism- degradation and biosynthesis of amino acids, sequence determination: chemical/ enzymatic/ mass spectral, racemization / detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).

#### b) Nucleic Acids

Purine and pyrimidine of nucleic acids, base pairing via H – bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acid (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis for heredity, an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and poly nucleosides.

#### **RECOMMENDED BOOKS:**

- 1. Principles of Biochemistry, A. L. Lehinger, Worth Publications.
- 2. Biochemistry, L. Stryer, W. H. Freeman
- 3. Biochemistry, J. David Rawn, Neil Patterson.
- 4. Biochemistry, Voet and Voet, John Wiley.
- 5. Outlines of Biochemistry, E. E. Conn and P. K. Stumpt, John Wiley.

# M.Sc. Part-II (Semester-IV) Organic Chemistry Practical Course OCHP-VII and OCHP-VIII

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#### Two or three stage preparations starting with 5g or less and TLC.

1. Estimation of Sulphur and Nitrogen.

#### **3.** Organic preparations (Any Five)

- 1. Preparation of Anthranilic acid.
- 2. Preparation of p- Amino benzoic acid.
- 3. Preparation of p- Chloro nitrobenzene by Sandmeyer reaction.
- 4. Preparation of p- Iodonitrobenzene by Sandmeyer reaction.
- 5. Preparation of Benzylamine
- 6. Preparation of Benzimidazole
- 7. Preparation of 2-acetyl cyclohexanone
- 8. Multicomponent synthesis.

**4. Project:** Literature survey. Study of reactions, synthesis, mechanism, isolation of natural products, standardization of reaction conditions, use of new methods etc. Identification of organic compounds by spectroscopic methods. External and internal examiners will examine the project (50 Marks) jointly at the time of practical examination.

### 5. Any other suitable experiments may be added.

# 6. Study tour may arrange for M.Sc. Part- II Students to visit Chemical Industries in nearby areas.

#### **REFERENCE BOOKS:**

- 1. A Textbook of Practical Organic Chemistry A. I. Vogel.
- 2. Practical Organic Chemistry Mann & Saunders
- 3. A Handbook of Quantitative & Qualitative Analysis- H. T. Clarke
- 4. Organic Synthesis Collective Volumes.

## M. Sc. Part II( Sem III and Sem IV) Physical Chemistry

#### SEMESTER- III

#### **CORE PAPERS**

- Paper –IX, PCH.3.1: Advanced Quantum ChemistryPaper –X, PCH.3.2: Electrochemistry
- Paper –XI, PCH.3.3 : Molecular Structure-I

#### **ELECTIVE PAPERS**

- Paper-XII(A), PCH.3.4(A) : Solid State Chemistry
- Paper -XII(B), PCH.3.4 (B) : Advanced Chemical Kinetics
- Paper -XII( C ), PCH.3.4(C) : Radiation and Photochemistry
- Practical Course : PCHP-V and PCHP-VI

#### **SEMESTER-IV**

### **CORE PAPERS**

Paper –XIII, PCH.4.1	: Thermodynamics and Molecular Modelling
Paper- XIV, PCH.4.2	: Chemical Kinetics
Paper- XV, PCH.4.3	: Molecular Structure II

# **ELECTIVE PAPERS**

Paper- XVI(A), PCH.4.4(A) : Surface Chemistry

Paper- XVI(B), PCH.4.4(B) : Chemistry of Materials

Paper- XVI(C), PCH.4.4(C): Biophysical Chemistry

Practical Course :PCHP-VII and PCHP-VIII

#### M.Sc. Part-II (Sem- III) Physical Chemistry

#### Paper -IX, PCH.3.1 : Advanced Quantum Chemistry

#### **Unit I: Basic Quantum Chemistry**

Introduction. Exact solution of Schrödinger wave equation for rigid rotator, linear harmonic oscillator and hydrogen and hydrogen like atoms. Atomic orbitals, radial and angular shapes of atomic orbitals, ground and excited state energies, ionization potentials for hydrogen like systems. Transition dipole moment integral and selection rules for rotational, vibrational and electronic transitions.

#### **Unit III: Ab initio methods**

Self-consistent field (SCF) theory, Hertree-Fock (HF) method, quantum particles and their spins, properties of slater determinant, HF equations, restricted Hartree-Fock (RHF) and unrestricted Hartree-Fock (UHF) models, Fock matrix, HF calculations, Roothan-Hall equations, Koopman's theorem, Basis sets: Slater type orbitals (STO), Gaussian type orbitals (GTO), difference between STO and GTO, energy calculations using such orbitals for multielectron systems, classification of basis sets, minimal basis sets, energy calculations for H-atom using STO basis sets at different levels, double- and triple-zeta basis sets, valence-split basis sets, polarized basis sets, truncation and superposition errors, methods to overcome these errors. Correlation energy.Post Hertree-Fock methods:Configuration interactions, many body perturbation theory, Möller-Plesset perturbation, coupled cluster method. Introduction to various software packages for performing ab initio calculations.

#### **Unit III: Density Functional Theory**

Basics of density functional theory (DFT): functionals, electron density and hole functions, fermi and coulomb holes, electron density as basic variable, Thomas-Fermi model, Slater's Approximation of Hartree-Fock Exchange, the Hohenberg-Kohn theorems, energy functionals, minimizing energy, orbitals and the non-interacting reference systems, the Kohn-Sham equations, computing the total energy, Exchange-Correlation energy functional, Solving the Kohn-Sham equations: basis sets, Pseudo-potentials, Plane waves, the self-consistent cycle,

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Density Functional Perturbation theory: basic formalism, first order energy derivative and atomic forces, second order.

#### **Unit IV: Semiempirical Methods**

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Introduction, need of semi-empirical methods, zero differential overlap (ZDO) approximation.Variation principle, Secular determinant and secular equations. Hamiltonian in semi-empirical methods, Hückel molecular orbital theory – Assumptions of HMO theory,  $\pi$ electron approximation, Hückel rule and aromaticity, HMO calculations for organic molecules, free valence index and prediction of chemical reactivity, use of molecular symmetry for simplification of HMO calculations. Neglect of differential overlap (NDO) method, complete neglect of differential overlap (CNDO), intermediate neglect of differential overlap (INDO), modified intermediate neglect of differential overlap (MINDO), modified neglect of differential overlap (MNDO), neglect of diatomic differential overlap (NDDO). AM1, PM3, PM5, PM6 etc. methods, comparisons in various above mentioned methods, limitations of semi-empirical methods. Introduction to various software packages for performing semi-empirical calculations.

#### **Reference Books:**

1. A.K. Chandra, Introductory Quantum Chemistry, 4th Edition, Tata McGraw-Hill, New Delhi, 1994.

2. D. A. McQuarrie, Quantum Chemistry, Viva Books, New Delhi, 2003.

3. P. Atkins and R. Friedman, Molecular Quantum Mechanics, 4th Edition, Oxford University Press, New York, 2005.

4. Leach, A.R. Molecular Modelling. Principles and Applications, 2nd Edition, Prentice-Hall, Harlow, England, 2001.

5. K.I. Ramachandran, G. Deepa and K. Nimboori, Computational Chemistry and Molecular Modelling: Principles and Applications, Springer-Verlag, Berlin, Germany, 2008.

6. Becker, O.; MacKerell, A.D.; Roux, B.; Watanabe, M. eds. Computational Biochemistry and Biophysics, Marcel Dekker, New York, 2001.

7. F. Jensen, Introduction to Computational Chemistry, 2nd Edition, John Wiley & Sons Ltd, West Sussex, England, 2007.

8. D.B. Cook, Handbook of Computational Chemistry, Oxford University Press, New York, 1998.

9. Fabio Finocchi, Density Functional Theory for Beginners: Basic Principles and Practical Approaches, 2011

10. Wolfram Koch, Max C. Holthausen, A Chemist's Guide toDensity Functional Theory, 2nd Edition, Wiley-VCH Verlag GmbH, Weinheim (Germany), 2001.

11. C. Fiolhais F. Nogueira M. Marques (Eds.), APrimer inDensityFunctional Theory, Springer-Verlag, Berlin, 2003.

12. P. Geerlings, F. De Proft, and W. Langenaeker, Conceptual Density Functional Theory, *Chem. Rev.* 2003, *103*, 1793-1873.

#### Paper – X, PCH.3.2: Electrochemistry

#### **UNIT-I: Equilibrium Properties of Electrolytes**

Non-ideal behaviour of electrolyte solutions, Debye – Huckel Theory of inter-ionic attraction, Ionic atmosphere, Time of relaxation, Relaxation and Electrophoretic effects, Debye – Huckel Onsagar equation, Validity of Debye – Huckel equation, factors influencing the degree of dissociation, , Debye – Falkenhagen effect, Wein effect, Debye Huckel limiting law equation, Qualitative and quantitative test of Debye Huckel limiting equation, Debye-Huckel Bronsted equations ,Ionic mobility, Determination of dissociation constant by emf method, Experimental determination of ionic mobility, osmotic coefficient, Bjerrum theory, association constant, Numerical problems.

#### **UNIT-II: Ion-solvent Interactions**

Structure of water, hydration, heats of hydration of electrolytes, individual ions and their comparison, calculation of heats of hydration( Born, Van Arkel & de Boer, Bernal-Fowler methods), entropy of hydration and hydration numbers. Ion transport in solutions, diffusion, chemical potential and work of transport, Ficks laws, expressions for flux and diffusion coefficient. Ionic liquids: Introduction, difference between electrolytes and ionic liquids, diffusion in fused salts, viscosity and diffusion coefficient in molten salts.

#### **UNIT-III: Electrode reactions**

Electrified interface, electron transfer under interfacial electric field, symmetry factor, electrode at equilibrium, exchange current density, over potential, Butler-Volmer equation, high field and low field approximations, Tafel equations, Multistep electrode reactions; Marcus microscopic model of electron transfer. Electrode kinetics of semiconductor/ solution interface; n and p type semiconductor, current-potential relation of n and p type semiconductors Electrocatalysis:

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Influence of various parameters on water splitting, HER and OER and Application of cyclic voltammetry for characterization of various electrochemical processes, Electrochemical instrumentations. Bioelectrochemistry: Nerve impulses, Membrane potentials, Nernst-Planck equation, Hodgkin-Huxley equations, electrochemical impedance spectroscopy.

#### **UNIT-IV: Fuel cell and Corrosion**

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**Fuel cell**: Significance of fuel cells, Hydrogen – oxygen fuel cells, hydrocarbon - air fuel cell, alkaline fuel cells, Phosphoric acid fuel cell (PAFC), Proton exchange membrane fuel cells (PEMFC), Solid oxide fuel cells, Molten Carbonate Fuel Cell (MCFC), Alkaline Fuel cell (AFC), Solid Polymer Fuel Cell (SPFC) and applications.

**Corrosion:** Introduction, Comparison between dry and wet corrosion, Factors affecting corrosion: Nature of the metal, Nature of the corroding environment, Types of corrosion, Prevention of corrosion: Material selection & Design, protective coatings, corrosion inhibitors.

#### **REFFERENCE BOOKS:**

1. An Introduction to Electrochemistry by Samuel Glasstone, East west press riveted limited. (2005).

2. Callister's Material Science and Engineering adapted by R. Balasubramaniam, Wiley India (p) Ltd.

3. Electrolytic Solutions, by R. A. Robinson and R. H. Strokes

4. Physical Chemistry by P. W. Atkins. ELBS.

5. Electrochemical Methods: Fundamentals and Applications, Bard, A. J. Faulkner, L. R., 2nd Ed., John Wiley & Sons: New York, (2002).

6. Electrochemical Science and Technology: Fundamentals and Applications, Oldham, K. B., Myland, J. C. and Bond, A. M. John Wiley & Sons, Ltd. (2012).

7. Modern Electrochemistry 2A: Fundamentals of Electrodics , 2nd Ed., Springer (2001).Bockris, J. O' M., Reddy, A. K. N. & Gamboa-Aldeco, M. E.

8 Electrochemistry, Brett, C. M. A. & Brett, A. M. O., Oxford University Press (1993).

9. Principles of Electrochemistry, John Wiley & Sons: NY (1993).

10. Fundamentals of electrochemistry, Bagotsky, V.S., 2nd Ed. Wiley – Interscience, (2006) Hamann, Carl H., Hamneff, Andrew & Vielstich, Wolf., Electrochemistry, 2nd Ed. (2007)

11. Fuel Cell Systems Explained Second Edition by James Larminie Andrew Dicks, John Wiley & Sons Ltd, The Atrium, Southern Gate, Chichester, West Sussex PO19 8SQ, England.

#### Paper -XI, PCH.3.3: Molecular Structure-I

#### UNIT- I: Symmetry properties of molecules and group theory (15)

Symmetry elements, symmetry operations and point groups, properties of group, symmetry operations as a group, multiplication table. Classes of symmetry operations, basis, representative and matrix representations of operations. Reducible and irreducible representations, orthogonality theorem. Properties of irreducible representations. Constructions of character table for point groups. Explanations for the complete character table for a point group. Representations of vibrational modes in nonlinear molecules. Infrared and Raman activities of normal modes of vibrations.

#### UNIT– II: Introduction of spectroscopy and Rotational Spectra (15)

Characterization of electromagnetic radiation. The qualification of energy. Regions of Spectrum, transition probability, the width and intensity of spectral transitions. Classification of molecules according to their moment of inertia. Rotational spectra of rigid and non rigid diatomic molecules. The intensities of spectral lines. The effect of isotopic substitution. Polyatomic and symmetric top molecules. The stark effect.

#### UNIT- III: Infrared spectroscopy and Raman Spectroscopy (15)

Diatomic molecules: 1) Molecules as harmonic oscillator, Morse potential energy function, vibrational spectrum, fundamental vibrational frequencies. Force constant, zero point energy, isotope effect. The anharmonic oscillator, the diatomic vibrating rotator, the interactions of rotations and vibrations. Polyatomic molecules: Fundamental vibrations and their symmetry, overtone and combination frequencies. The influence of rotations and molecular spin on the spectra of polyatomic molecules. Analysis by Infrared techniques. Raman Spectroscopy:

Rayleigh scattering. Raman Scattering, classical and quantum theories of Raman effect. Rotational Raman Spectra for linear and symmetric top molecules. Vibrational Raman Spectra, rotational fine structure. Polarization of light and the Raman effect . Structure determination from Raman and Infra-red spectroscopy.

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#### **UNIT – IV: Electronic Spectroscopy**

General nature of band spectra. Beer- Lambert Law integrated absorption coefficient and oscillator strength. Term symbols for atoms and molecules. The hydrogen atom and hydrogen like species spectrum. Sequences and progressions, the vibrational course structure and rotational fine structure of electronic band. The Franck-Condon principle, dissociation energy and dissociation products. Birje-Sponer extrapolation. The fortrat diagram. Predissociation, classification of electronic states. The spectrum of molecular hydrogen. Electronic spectra of polyatomic molecules. Chemical analysis by electronic spectroscopy. (d-d), ) and  $(\neg-n^*)$  transitions. Photochemical mechanism of vision.

#### **REFFERENCE BOOKS:**

1. Fundamental of molecular spectroscopy by C. N. Banwell, E. M. McCash, Vth Edn.,

Tata McGrew Hill(2013).

2. Physical Chemistry by P. W. Atkins, J. D. Paula, IXth Edn., Oxford University Press (2010).

3. Chemical Applications of Group Theory, F. A. Cotton, 3rd Edn., Wiley-India(2009).

4. Molecular Symmetry and Group Theory by R. L. Carter, John-Wiley & Sons Inc.(1998)

5. A Text Book of Physical Chemistry by K. L. Kapoor, IVth Edn., Macmillan (2011).

6. Symmetry & spectroscopy of molecules by K. Veera Reddy, IInd revised Edn., New Age International Publishers (2009)

7. Intruduction to spectroscopy by D. L. Pavia, G. M. Lapmann, G. S. Kriz, IIIrd Edn., Thomson(2006).

8. Molecular Structure and Spectroscopy by G. L. Aruldhas, Prentice-Hall of India Pvt. Ltd. (2006).

#### Paper XII (A), PCH-3.4(A): Solid State Chemistry (Elective)

#### **UNIT-I:** The solid state

Introduction, laws of crystallography, lattice types, X-ray diffraction, Bragg's equation, Miller indices, Bragg Method, Debye-Sherrer method of X-ray structure analysis of crystals, indexing of reflections, identification of unit cells from systematic absence in diffraction pattern, structure of simple lattice and X-Ray intensities, structure factor and its relation to intensity and electron density, phase problem, procedure for an X-ray structure determination.

#### **UNIT –II: Solid State Reactions**

General principle, types of reactions: Additive, structure sensitive, Decomposition and phase transition reactions, tarnish reactions, kinetics of solid state reactions, factors affecting the reactivity of solid state reactions.

#### **UNIT –III: Electronic Properties and Band Theory**

Metals, insulators and semi conductors, free electron theory and its applications, electronic structure of solids, band theory, band structure of metals, insulator, and semiconductors, doping in semiconductors, p-n junction, superconductors, Molecular materials, Organic materials, some examples of organic semiconductors, charge carrier injection and transport, Optical properties of organic semiconductors, applications and devices involving optical properties, luminescence photoluminescence, effect of impurity levels on photoluminescence, light emitting diodes, luminous efficiency, photo-conduction and photoelectric effects, laser, principle of laser action, solid state laser and their applications.

#### **UNIT-IV: Preparation of materials**

Purification and crystal growth, kinetics of nucleation, radius of nucleus, critical radius, principle of nucleation, crystal growth during casting, zone refining, growth from solution, growth from melt and preparation of organic semiconductors for device applications.

#### **Crystal Defect and Non Stiochiometry**

Classification of defects subatomic, atomic and lattice defect in solids. Thermodynamics of vacancy in metals, Thermodynamics of Schottky defects in ionic solids, Thermodynamics of Frenkel defects in silver halides. Calcualtion of number of defects and average energy required for defect.

#### **REFERENCE BOOKS:**

- 1. A guide to laser in chemistry by Gerald R., Van Hecke, Keny K. Karokitis
- 2. Principals of solid state, H. V. Keer, Wiley Eastern,
- 3. Solid state chemistry, N. B. Hannay
- 4. Solid state chemistry, D. K. Chakrabarty, New Age International
- 5. An Introduction to Crystallography : F. G. Philips
- 6. Crystal Structure Analysis: M. J. Buerger

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7. The Structure and properties of materials:

Vol. III Electronic properties by John Walss

8. Electronic processes in materials : L. U. Azroff and J. J. Brophy

9. Chemistry of imperfect crystal : F. A. Krogen

10. Elements of X-ray Diffraction by B. D. Cullity, Addison- Weily.

11. Solid state Chemistry by A.R.West (Plenum)

12. Electronics made simple by Jacobwitz.

13. Principles of Physical Metallurgy, by Abhijeet Mallick,

14. Solid State Chemistry, An Introduction, by Lesley E. Smart, & Elaine A. Moore,

Third Edition, Taylor & Francis, Indian Edition 2012.

#### Paper XII (B), PCH-3.4(B): Advanced Chemical Kinetics (Elective)

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#### Unit-I: Hydrogen ion dependence of reaction rates:

Protonation and hydrolysis equilibria, determination of active reactant species form kinetic data, interpretation of hydrogen ion effect with example.

#### Unit-II: Electron transfer reaction:

Complimentary and non-complimentary reactions, outer and inner-sphere electron transfer reactions, proton transfer, hydride transfer and hydrogen, oxygen and chlorine atom transfer reactions.

#### **Unit-III: Catalysis:**

Trace metal ion catalysis and their mechanisms. Micellar catalysis, Berezini, Menger-Portonoy, cooperative and pseudo-phase ion exchange models and examples.

#### Unit-IV: Mechanism of chromium (VI) oxidations:

One and two equivalent reductants oxidation, assumptions, limiting forms of rate laws, Westheimer mechanism and its validity. Catalysis, Induced and cooxidations. Mechanisms other than Westheimer mechanism.

#### **REFERENCE BOOKS AND ARTICLES**

1) Chemical Kinetics by K. J. Laidler.

2) Kinetics and Mechanism by A. A. Frost and R. G. Pearson

3) Micellar effect on the kinetics and mechanism of chromium(VI) oxidation of organic

substrates By Asim K. Das, Coordination Chemistry Reviews, Vol 248, p 81-89 (2004).

4) Some aspects of electron transfer reactions involving organic molecules by B. Sethuram, Allied Publishers, 2003.

5) Surfactants and polymers in aqueous solution by Bo Jonsson, Bjorn Lindman, Krister Holmberg and Bengt Kronberg, John-Wiley & Sons, 1998.

6) Inorganic reaction mechanisms, Part II Edited by John O. Edwards, Interscience, 1972.

#### Paper XII (C), PCH-3.4(C) : Radiation and Photochemistry(Elective)

#### **Unit - I : Radiation Chemistry :**

Introduction, Radiation Types, their characteristics, Radiation in chemical processes.

#### Unit - II: Lasers and Lasers in Chemistry :

Introduction, characteristics of laser, uses of lasers in chemical process, laser induced chemical reactions, organic photochemistry, lasers as a photochemical tool, laser induced selective bond chemistry, overview, bond selective chemistry of light atom molecules.

#### Unit - III: Basics of Photochemistry :

Electrochemistry of excited states, life time measurements, flash photolysis, energy dissipation by radiative and non-radiative processes, properties of excited states, structure, dipole moment, acid-base strength, reactivity, photochemical kinetics, calculations of rates of radiative process, bimolecular quenching, Luminescence for sensors and switches, charge transfer excited state, photoinduced electron transfer reactions.

#### Unit - IV : Micellaneous Photochemical reaction :

Photo-fries reaction of anilides , photo - fries rearrangement, Barton reaction , singlet molecular oxygen reactions , photochemical formation of smog , photodegradation of polymers , photochemistry of vision .

#### **REFRENCE BOOKS**

1) Molecular Photochemistry, N. J. Turro, W.A. Benjamin

2) Fundaments of Photochemistry, K. K. Rohatagi - Mukherji, Weiley - Eastern

3) Elements of Inorganic Photochemistry : G. S. Ferraudi , Wiley

4) Concepts of Inorganic Photochemistry, A.W. Adamson & P. J. Fleischauer, Wiley

5) A Guide To lasers in chemistry, Gerald R. Van Hecke & Kerry K. Karukstis.

6) Photochemistry, R.P. Kundall, A Gilbert, Thomson Nelson

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# M.Sc. Part-II (Semester-III) Physical Chemistry Practical Course PCHP-V and PCHP-VI

- 1) Determination of stability constant of ferric thiocyanate complex.
- To determine stoichiometry and stability constant of ferric-salicylate complex by Job's Method and mole ratio method spectrophotometrically.
- 3) Determination of stoichiometry and instability constant silver ammonia complex.
- 4) Determination of transport number of H<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup> etc. ions using moving boundary method
- 5) Determination of the critical micelle concentration of a given surfactant in aqueous and aqueous salt solutions.
- 6) Determination of equivalent conductance at infinite dilution and dissociation constant for weak acid using Kolharausch Law of independent ionic mobility.
- 7) pH-metric determination of dissociation constant of carbonic acid.
- Cryoscopic determination of molecular weight and state of organic acids in nonaqueous volatile solvents.
- Determination of order of reaction for iodination of acetone catalyzed by acid with reference to acetone, iodine and acid catalyst.
- 10) Determination of apparent and partial molar volumes of 1:1 electrolytes in aqueous solutions using pyknometric method of density measurements.
- Structure drawing, Geometry optimization and Single-point energy calculations for small molecules using minimal basis sets.
- 12) Structure drawing, Geometry optimization and Single-point energy calculations for small molecules using correlation consistent basis sets.
- Semi-empirical and quantum mechanical determination of thermochemical properties of small molecules.

#### M.Sc. Part-II (Sem- IV) Physical Chemistry

#### Paper -XIII, PCH.4.1: Thermodynamics and Molecular Modelling

#### **Unit I: Modern Theoretical Principles**

Exact and inexact differential expressions in two variables. Total differentials. Techniques of partial differentiations. Transformation of variables. Maxima and mimima. Integrating factors, Paff differential equations, Caratheodary's theorem. Legendre transformations. Derivation of thermodynamic identities. The second law of thermodynamics, classical formulations, mathematical consequences of second law. Entropy changes, Clausius inequality. Free energy concept. General condition of equilibrium. Thermodynamic potentials.

#### **Unit II: Statistical Thermodynamics**

Ensembles, ensemble average and time average of the property, ergodic hypothesis, partition functions and thermodynamic properties, classical and quantum statistics, properties of photon gas, thermodynamic properties bosons, use of quantum statistics for evaluation of absolute entropies, condensation of helium, Fermi energy, electron gas in metals.Heat capacity of solids, Einstein and Debye specific heat equations. Characteristic temperatures. Debye  $T^3$  law.

#### Unit III: Molecular Mechanics and Molecular Dynamic Simulation Methods (15)

Introduction, microscopic and macroscopic properties, time scale of chemical/biological process, the Morse potential model, harmonic oscillator model, force fields development, various energy terms and non-covalent interactions included in force fields, Lennrad-Jones type and truncated Lennard-Jones potentials, commonly used force fields, parameterization, advantages and limitations of Force Field Methods, molecular dynamics methods, neighbour searching, Trotter decomposition, cut-offs, temperature and pressure coupling methods, integration algorithms: Verlet algorithm, Leap-frog algorithm, Velocity Verlet, Beeman's algorithm, Constraint algorithms: shake, lincs, etc., topology files, energy minimization: steepest descent method, conjugate gradient method, L-BFGS. Solvent models, Solvation, implicit and explicit solvation, heating dynamics, equilibration dynamics, production dynamics, trajectory analysis, particle mesh Edward dynamics, boundary conditions, Exclusions and 1-4 interactions, replica exchange method, conformational analysis, normal mode analysis, free energy calculation: free energy perturbation method, thermodynamic integration method, thermodynamic cycles for free energy calculations, determination of hydration/solvation free energy, protein folding free energy, protein-ligand binding free energy etc. Software packages for performing Molecular dynamic simulation as well as for visualization and analysis trajectories

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#### Unit IV: Non-equilibrium thermodynamics

Conversion of mass in closed and open systems, conservation of energy in closed and open systems. Law of increasing entropy. Non-adiabatic process and clausius inequality, steady state. Thermodynamic equations of motion. Chemical and electrochemical affinities. Coupling reactions. Rates and affinities. Generalized fluxes, forces and their transformation. Phenomenological equations and coefficients. Concepts of reciprocity relations and Onsager theorem of microscopic reversibility. Entropy production in closed and open systems. Entropy production due to heat flow. Chemical potentials. Diffusion, electromotive force, electroosmosis, thermoelectric effect and other reactions involving cross relations. Saxen's relations.

#### **Reference Books:**

1. S. N. Blinder, Advanced physical Chemistry, The Macmilan Company, 1967.

2. L. K. Nash, Elements of statistical thermodynamics, 2nd Edition, Addison Wesley, 1974.

3. T.L. Hill, An Introduction to Statistical Thermodynamics, Addison-Wesley, 1960.

4. S. Glasstone, Theoretical Chemistry: An introduction to quantum mechanics, statistical mechanics, and molecular spectra for chemists, D. Van Nostrand Company, Inc., 1944.

5. D. A. McQuarrie and J. D. Simon, Physical Chemistry: A molecular Approach, Viva Books, New Delhi, 1998.

6. Allen, M. P., Tildesley, D. J. Computer Simulations of Liquids, Oxford: Oxford Science Publications. 1987.

7. Frenkel, D.; Smit, B. Understanding Molecular Simulation: From Algorithms to Applications, 2nd Edition, Academic Press, San Diego, 2002.

8. K.I. Ramachandran, G. Deepa and K. Nimboori, Computational Chemistry and Molecular Modelling: Principles and Applications, Springer-Verlag, Berlin, Germany, 2008.

9. F. Jensen, Introduction to Computational Chemistry, 2nd Edition, John Wiley & Sons Ltd, West Sussex, England, 2007.

10. Schlick, T. Molecular modeling and simulation: an interdisciplinary guide, Springer-Verlag New York, Inc., Secaucus, NJ, USA, 2002.

 D.B. Cook, Handbook of Computational Chemistry, Oxford University Press, New York, 1998.

12. Online Manuals for simulation and visualization packages such as GROMACS, VMD, NAMD, AMBER, TINKER, etc.

13. I. Prigogine, Introduction to Thermodynamics of Irreversible Processes, Wiley, New York, 1968.

14. R.P. Rastogi, Introduction to Non-equilibrium Physical Chemistry: Towards Complexity and Non-linear Science, Elsevier, Oxford, 2008.

#### Paper- XIV, PCH.4.2: Chemical Kinetics

#### **UNIT-I:** Collision Theory

Collision Theory: Definition, Formulation of the total collision rate, The p factor, Reactive collisions, Contour diagrams for scattering of products of a reaction, Forward scattering: the

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stripping or grazing mechanism, Backward scattering: the rebound mechanism, Scattering diagrams for long-lived complexes, Steady State Approximation Collision theory of gas reaction, collision frequency. The rate constant, molecular diameters, collision theory vs. experiment

#### **UNIT – II: Transition State Theory**

Transition State Theory: Transition state theory, configuration and potential energy, Properties of the potential energy surface relevant to transition state theory, An outline of arguments involved in the derivation of the rate equation, Use of the statistical mechanical form of transition state theory, Comparisons with collision theory and experimental data. Thermodynamic Formulations of Transition State Theory: Determination of thermodynamic functions for activation, the partition function form and the Thermodynamic form of transition state theory, Typical approximate values of contributions entering the sign and magnitude of  $\Delta S^{\#}$ , Unimolecular Theory: Manipulation of experimental results, Physical significance of the constancy or otherwise of k<sub>1</sub>, k<sub>-1</sub> and k<sub>2</sub>, Physical significance of the critical energy in unimolecular reactions, Physical significance of the rate constants k<sub>1</sub>, k<sub>-1</sub> and k<sub>2</sub>. Lindemann, Hinshelwood, theory, Kassel and Slater Theory.

#### **UNIT-III: Kinetics of Surface Reactions**

Review of adsorption isotherms, Thermodynamics and statistical mechanics of adsorption, Structure of soilid surfaces and adsorbed layers: Detailed structural studies, Induced Heterogenity, Mechanism of surface reactions: Kinetic effects of surface heterogeneity, Kinetic effects of interaction Unimolecular surface reactions: Inhibition, Activation Energies, Bimolecular surface reactions: Reaction between two adsorbed moleculesreaction between a gas molecule and an adsorbed molecule, Adsoprtion of two gases without mutual displacement, Inhibition, Activation energies, Parahydrogen conversion, Combination and formation of atoms at surfaces, Exchange reactions,Addition of hydrogen to ethylene, Transition state theory of surface reactions: rates of chemisorptions, rates of desorption, Unimolecular surface reactions,bimolecular surface reactions,comparison of homogeneous and heterogeneous reaction rates, Problems

#### UNIT- IV : Fast Reactions and Organic Reaction Mechanisms (15)

Linear free energy relationships: Hammett plots Hammett equation, substituent and reaction constants and their physical significance, calculation of k and K values, Yukawa-Tsunoequation.Taft equation, steric parameters Solvent effects, Grunwald-Winstein equation.

Kinetics of Fast reactions: Relaxation techniques, pressure jump and temperature jump methods, NMR relaxation, flash photolysis and molecular beam methods.

#### **REFERENCE BOOKS**:

- 1) Chemical Kinetics by K. J. Laidler, Third Edition, Pearson.
- 2) Kinetics and Mechanismby A. A. Frost and R. G. Pearson.
- 3) Fast Reactions by Haque.

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4) Theory of chemical reaction rates by K. J. Laidler, McGrew Hill, New York, 1969.

- 5) Fast Reactions by J. N. Bradley, Clarendon Press Oxford, 1974
- 6) Physical Chemistry by W. J. Moore.

7) Physical Chemistry by P.W. Atkins

8) Mechanism of Inorganic Reactions by F. Basolo and R. G. Pearson, John Wiley

& Sons Inc., 2nd Edition, 1967.

9) A Guidebook to Mechanism in Organic Chemistry, Peter Sykes, Orient Longmann, 6th Edition, 2003.

#### Paper- XV, PCH.4.3: Molecular Structure - II

#### UNIT – I: The Electrical and Magnetic Properties of Molecules

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Electric dipole moment of molecule, polarization of a dielectric, polarizability of molecules, Clausius-Mossotti equation. Debye equation. limitation of the Debye theory, determination of dipole moment from dielectric measurements in pure liquids and in solutions.

Diamagnetism and paramagnetism. Volume and mass susceptibilities. Lengevins classical theory of diamagnetism and paramangnetism Atomic and ionic susceptibility. Pascal constants, Curie - Weiss law. Van Vleck general equation of magnetic susceptibility. Determination of magnetic susceptibility.

CO: the unit deals with the understanding of behaviour of various materials in presence of applied electrical and magnetic fields.

#### UNIT – II: Nuclear Magnetic Resonance Spectroscopy

The nature of spinning particles , interaction between spin and a magnetic field. Population of energy levels, The larmor precession . relaxation times. the meaning of resonance and the resonance condition. NMR experiment, singnificance of shielding constants and chemical shift . the origin and effect spin - spin coupling , factors affecting chemical shift, chemical analysis by NMR. Exchange phenomena , 13C NMR spectroscopy, double resonance and nuclear-overhauser effect.

CO: the student will be able to predict structure of the given compound.

#### UNIT – III: Electron Spin Resonance Spectroscopy and Massbauer Spectroscopy (15)

Electron spin and Magnetic moment, Resonance condition in ESR and significance of 'g' value. ESR spectra of organic free radicals, McConnel relation, Electron Exchange reactions, applications of ESR, B) Massbauer Spectroscopy (7) Basic principle of Mossbauer spectroscopy, hyperfine structure, quadrupole splitting, instrumentation and applications of Mossbauer spectroscopy, Problems related to Mossbaur spectra.

CO; the student will be able to understand behaviour of electrons and nucleus of a given molecule in presence of an external force like magnetic field.

#### UNIT - IV: Basics of Fluorescence Spectroscopy

Photoluminescence, Instrumentation, Electronic transition in atoms and molecules, Solvatochromism, Fate of excited molecules, structural factors, properties of fluorescence, Fluorescence parameters: fluorescence intensity, quantum yield and fluorescence life time, Corrected emission and excitation spectrum, Relation between emission spectrum and excitation spectrum, inner filter effect, Solvent effect on fluorescence, solvation dynamics, Effect of intermolecular process, Fluorescence Anisotropy, Relation between concentration with fluorescence and phosphorescence intensity, Fluorescence quenching, Energy transfer, Excited state proton transfer, Synchronous spectrum, Fluorescent nanomaterials and its applications.

#### **REFFERNCE BOOKS:**

1.Fundamental of molecular spectroscopy by C. N. Banwell, E. M. McCash, Vth Edn., Tata McGrew Hill(2013).

- 2. Physical Chemistry by P. W. Atkins, J. D. Paula, IXth Edn., Oxford University Press (2010).
- 3. Introduction to molecular spectroscopy by G. M. Barrow.
- 4. Molecular spectroscopy by I. N. Levins, Wiley interscience.
- 5. Nuclear magnetic Resonance by J. D. Roberts, Mcgrew Hill.
- 6. Introduction to Magnetic resonance by A. Carrrington and A. D. McLachlan. Harper and Row.
- 7. Intruduction to spectroscopy by D. L. Pavia, G. M. Lapmann, G. S. Kriz, IIIrd Edn., Thomson(2006).
- 8. Introduction to Magnetochemistry by Earnst Shaw. Academic Press
- 9. Electrical and optical properties of molecular behavior by M. Davies, Pergmon press.
- 10. Polar molecules by P. Debye, Dover publications.
- 11. A Text Book of Physical Chemistry by K. L. Kapoor, IVth Edn., Macmillan (2011).
- 12. Principles of Fluorescence Spectroscopy, 3<sup>rd</sup> edition, Joseph R. Lakowicz (Springer)
- 13. Fundamentals of Photochemistry by K. K. Rohatgi-Mukherjee

14. Molecular Fluorescence: Principles and Applications. Bernard Valeur, 2001, Wiley-VCH Verlag GmbH

#### Paper- XVI (A), PCH.4.4(A) : Surface Chemistry (Elective)

#### **UNIT-I: Surface Chemistry of interfaces**

Types of interfaces, Liquid-vapour interface, Surface tension and interfacial tension, surface tension across curved surfaces, capillary action, methods of determination of surface tension, , vapor pressure of droplet (Kelvin equation), Surface activity and adsorption phenomenon, Trube's Rule, liquid-liquid interfaces, work of cohesion and adhesion, surface spreading , spreading of one liquid on the surface of other liquid, spreading coefficient and derivation for its relation with surface tension, surface films on liquids, criteria for spreading of one liquid on

another. Experimental techniques for the study of monomolecular films, states of monomolecular films reaction on monomolecular films, catalytic activity at surfaces.

#### UNIT -II: Solid-Liquid and Solid - Solid interfaces

Solid-liquid interfaces, Introduction, wetting phenomenon, contact angle and wetting, heat of wetting, methods of determination of contact angle, contact angle hysteresis, wetting agents, selective wetting, applications in detergency, and pesticide affectivity, Solid-Solid interfaces, introduction, Surface energy of solids, adhesion and adsorption, sintering and sintering mechanism, Tammann temperature, importance of impurities, surface structure and surface composition. Friction and lubrication, mechanism of lubrication, solid state lubricants.

#### **Unit-III: Solid-gas interfaces**

Adsorption, Mechanism of adsorption, Adsorption of gases by solids, Factors affecting adsorption, Characteristics, Experimental methods of determining gases adsorption, Adsorption of solutes from solution, Heat of adsorption, Measurement of heat of adsorption, Chemisorption: kinetics of chemisorption, heat of chemisorptions, Surface film, Catalysis of gases reaction by solid surface, One reactant gases slightly/ strongly/ moderately adsorbed, Retarded reaction, ion exchange adsorption, Applications

#### **UNIT- IV: Colloids and emulsion**

Colloidal solution, classification of colloids, Theories of origin of charge on sol particles, Determination of charge on a colloidal particle, Stability of sols, Association colloids, Spontaneous ageing of colloids, Factors affecting the spontaneous ageing, theories of spontaneous ageing, coagulation, kinetics of coagulation.

**Emulsion**: Types of emulsion, preparation, properties, Characteristics, Identification test between two types of emulsions, emulsifiers, demulsification. Gels: classification, methods for the preparation of gels, properties of gels, Applications of colloid science.

#### **REFFERNCE BOOKS:**

- 1. Physical chemistry of surfaces: A. W. Adamson.
- 2. Introduction to colloid and surface chemistry by D. J. Shaw.

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3. Surface chemistry by J. J. Bikermann

4. The Surface Chemistry of Solids, by S.J. Gregg, Second Edition, Chapman & Hall Ltd. London.

5. Advanced Physical Chemistry, by Gurdeep Raj ,Goel Publishing House, Krishna Prakashn Media (P) Ltd., Meerut-250001(UP)

6. Physical Chemistry by Pahari S. New Central Book Agency (P) Ltd. Kolkata700009.

- 7. Advanced Physical Chemistry J.N. Gurtu, A. Gurtu. 11th Edition Pragati Prakashan.
- 8. Advanced Physical Chemistry D N Bajpai S Chand Publications
- 8. Essentials of Physical Chemistry by Arun Bahl, B S Bahl, G D Tuli . S Chand Publications
- 9. Principles of Physical Chemistry by S H Maron and C F Prutton

#### Paper- XVI (B), PCH.4.4(B) : Chemistry of Materials (Elective)

#### Unit I: Glasses, Ceramics, Composite and Nanomaterials:

Glassy state, glass formers and glass modifiers, applications, Ceramic structures, mechanical properties, clay products. Reformatories, characterizations, properties and applications. Microscopic composites; dispersion - strengthened and particle - reinforced, fibre - reinforced composites, macroscopic composites. Nanocrystline phase, preparation procedures, special properties, and applications.

#### Unit II: High Tc Materials:

Defect perovskites, high Tc superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, and normal state properties; anisotropy; temperature dependence of electrical resistance; optical photon modes, superconducting state; heat capacity; coherence length, elastic constants, position lifetimes, microwave absorption - pairing and multigap structure in high Tc materials, applications of high Tc materials.

#### **Unit III: Polymeric Materials:**

Molecular shape, structure and configuration, crystallinity, stress- strain behavior, thermal behavior, polymer types and their applications, conducting and ferro - electric polymers.

#### Unit IV: Materials of Solid Devices:

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**a)Thin films and Langmuir- Blodgett Films:** Preparation techniques; evaporation / sputtering, chemical processes, MOCVD, sol - gel etc. Langmuir- Blodgett (LB) film, growth techniques, photolithography, properties and application of thin and LB films.

**b)** Materials of Solid Devices: Rectifiers, transistors, capacitors IV-V compounds, low dimensional quantum structure; optical properties.

#### **REFFERNCE BOOKS**

1. Solid State Physics, N. W. Ashcrott and N. D. Mermin, Saunders College

2. Material Science and Engineering, An introduction, W. D. Callister, Willey.

3. Principals of Solid State, H. V. keer, Willey Eastorn.

4. Materials Science , J. C. Anderson , K. D. Leaver, J. M. Alexander and R. D. Rawlings, ELBS

5. Thermotropic Liquid Crystals, Ed, G. W. Gray, John Willey.

6. Text book of liquid crystals, Kelkar and Halz, Chemie Verlag.

#### Paper- XVI (C), PCH.4.4(C): Biophysical Chemistry (Elective)

#### Unit - I Chemistry and Biology:

Amino acids, proteins, enzymes, DNA & RNA in living systems, electrolytes, the chirality of biological molecules, the biochemical process, weak and strong interactions, macromolecules and rubber elasticity, polyelectrolytes, biopolymers.

#### Unit - II Physical aspects of biopolymers:

X-ray diffraction, electronic absorption & luminescence Spectroscopy, optical activity, magnetic activity, magnetic-optical activity. Osmosis, hydrophobic hydration and interactions. The properties of amino acids and their aqueous solutions.

#### **Unit - III Photo biological Process :**

Photosynthesis, mechanism of vision, the molecular mechanism of photoreceptor.

#### Unit - I : Mechano-chemical processes :

Introduction, thermodynamics, nerve conduction and membrane equilibria, muscle and muscle proteins, their chemistry and physics, kinetic properties of muscle, mechano- chemical systems, biomachanics.

#### **REFFERENCE BOOKS**

1) Biophysics by M.V. Volhenshfein.

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2) Natural products : Chemistry & Biological Significance, J. Mann, R.S.

Davidson, J. B. Hobb's , D. V. Banthrope and J. B. Harborne , Longmar Essex

3) Elements of Inorganic Photochemistry, G. J. Ferrandi, wiley

4) Principals of bioinorganic chemistry , S. J. Lippard and J. M. Beng , University Science Books,

5) Principals of biochemistry, A. L. Lechinger, worth publisher

6) Biochemistry, J. David Rawn, Neil Patterson

7) Hydrophobic interactions by Ben-Naim, Plenum.

# M.Sc. Part-II (Semester-IV) Physical Chemistry Practical Course PCHP-VII and PCHP-VIII

#### Practical courses includes Submission of project work :

- Statistical representation of given experimental data: Estimation of errors in measured and derived properties, reporting data with appropriate significant figures, graphical representation of data with x- and y-error bars.
- Determination of molecular properties of small gaseous molecules from rovibrational spectra.
- 3) Determination of indicator constant and isosbestic point of an indicator.
- 4) Determination of Thermodynamic Parameters for electrochemical reactions: To determine  $\Delta G^0$ ,  $\Delta H^0$  and  $\Delta S^0$  for the formation of 1 mole of cadmium in 1 wt. % amalgam at 25 °C.
- 5) Determination of isoeletric points and dissociation constants for netutral, acidic and basic amino acids using pH-metric technique.

- 6) Cryoscopic determination of mean activity coefficient of 1:1 electrolytes in aqueous solutions.
- Study of the effect of ionic strength on the reaction between persulphate and iodide by visual method.
- 8) Determination of molar enthalpy of solution, molar enthalpy of dilution and partial molar heat content of components in aqueous solutions.
- Structure drawing, Geometry optimization and Single-point energy calculations for small molecules using minimal basis sets.
- Structure drawing, Geometry optimization and Single-point energy calculations for small molecules using correlation consistent basis sets.
- 11) Electronic structure calculations for small molecules and their aggregates.
- 12) Calculation of vibration spectra using *abinitio* techniques.
- 13) Structure and properties of transition states from DFT calculation.
- Determination of thermodynamic properties from Molecular dynamic simulations of some simple systems.

Along-with above experimental and computational lab work, additional new experiments from computational chemistry as well as from experimental techniques will be given whenever required and found necessary for enhancing the knowledge and skill of the students. A research project is compulsory for each student. Project shall be started at the beginning of Sem – III and will be accessed bimonthly for its progress and continuous evaluation will be made. High standard research work is expected from the project and students are encouraged to publish it in national or international journals of high repute.

Study tour is compulsory for M.Sc. Part- II Students to visit Chemical Industries in India.

#### M.Sc. Part-II, (Sem-III IV) Analytical Chemistry

#### **SEMESTER-III**

Paper No. – IX, ACH 3.1	: Advanced Analytical Techniques
Paper No. – X, ACH 3.2	: Organo Analytical Chemistry
Paper No. – XI, ACH 3.3	: Electroanalytical Techniques in Chemical Analysis

#### **ELECTIVE PAPERS**

<b>Paper No.</b> –XII (A), ACH 3.4(A)
Paper No XII (B), ACH 3.4(B)
<b>Paper No.</b> – XII(C), ACH 3.4(C)

: Environmental Chemical Analysis and Control : Recent Advances in Analytical Chemistry : Chemical Analysis in Agro, Food and Pharmaceutical Industries : ACHP-V and ACHP-VI

Practical Course

#### **SEMESTER-IV**

**Paper No.** – XIII, ACH 4.1 Paper No. – XIV, ACH 4.2 **Paper No.** – XV, ACH 4.3 **ELECTIVE PAPERS Paper No.** – XVI (A), ACH 4.4(A) : Applied Analytical Chemistry **Paper No.** - XVI (B), ACH 4.4(B) **Paper No.** - XVI (C), ACH 4.4(C)

- : Modern Separation Method in Analysis
- : Organic Industrial Analysis
- : Advanced Methods in Chemical Analysis
- : Quality Assurance and Accreditation

: Techniques in Forensic Sciences and Microbiological Analysis

#### : ACHP - VII and ACHP-VIII

**Practical Course** 

#### M.Sc. Part-II (Sem-III) Analytical Chemistry

#### Paper No. -IX, ACH 3.1: ADVANCED ANALYTCAL TECHNIQUES

#### **UNIT-I:** Advances in Mass Spectrometry-A

Introduction to Mass spectrometry, diagram of a mass spectrometer and Instrumentation, principles, history, concept of ion free path, classification of mass spectrometry based on nature of compound to be analyzed and the ion sources viz. Electron impact (EI), chemical ionization (CI), Fast ion or atom bombardment ionization (FID/FAB), field desorption (FD), laser desorption ionization (LDI), plasma desorption ionization (PDI), thermospray ionization (TSI), electrospray (ESI), atmospheric pressure ionization, Inductively couple plasma (ICP) etc. Mass Analyzers, Quadrupolar Analyzers, Quadrupole ion trap or Quistor, Ion trap detector, development of high –Mass, High-resolution ion trap, tandem mass spectrometry in the ion trap, time of flight analyzer, magnetic and electromagnetic analyzer, ion cyclotron resonance and FT-MS, and detectors

#### UNIT-II: Introduction to Nanotechnology and Nano Chemistry

Definition of nanomaterials and nanotechnology, significance of nanotechnology, size and properties, types of nanomaterials like 0D (quantum dots), 1D, 2D and 3D, introduction to physical, chemical and biological synthesis of nanomaterials with suitable examples, top down and bottom-up approach, chemical synthesis of nanomaterials-Different types and processes for synthesis of nanomaterials using wet chemical approaches. Fabricating nanomaterials with different morphology intended for specific applications. Applications of Nanotechnology.

#### **UNIT-III: Advanced Instrumentation Techniques-A**

Scanning Electron Microscope (SEM) - Introduction, principle, instrumentation, applications Transmission Electron Microscope (TEM) - Introduction, principle, instrumentation, applications Electron Dispersion Spectroscopy (EDS) - Introduction, principle, instrumentation, applications Energy Dispersive X-ray Analysis (EDAX) - Introduction, principle, instrumentation, applications

Scanning Tunneling Microscopy (STM) - Introduction, principle, instrumentation, applications Atomic Force Microscopy (AFM) - Introduction, principle, instrumentation, applications Practical applications and examples in analytical chemistry and research.

#### **UNIT-IV: Advanced Instrumentation Techniques-B**

Raman Spectroscopy- Introduction, principle, instrumentation, applications

X-Ray Fluorescence Spectroscopy (XFS) - Introduction, principle, instrumentation, applications Electron Spin Resonance Spectroscopy (ESR)- Introduction, principle, instrumentation, applications

X-Ray Photoelectron Spectroscopy (XPS)- Introduction, principle, instrumentation, applications Auger Electron Spectroscopy - Introduction, principle, instrumentation, applications

Secondary Ion Mass Spectrometry (SIMS)- Introduction, principle, instrumentation, applications Practical applications and examples in analytical chemistry and research.

#### **Recommended Books:**

1) E. De. Hoffmann, J. Charette, V. Stroobant, Mass Spectroscopy: Principles and Applications, John Wiley & Sons, Masson, Paris 1996.

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- 2) J. H. Gross, Mass Spectroscopy: A Text book, Springer-Verlag Berlin 2004.
- 3) C. G. Herbert, R. A. W. Johnstone, Mass Spectrometry Basics, CRC Press, Boca Raton, Florida, 2002.
- 4) K. Benjamin : Mass Spectrometry
- 5)
- 6) A. I. Vogel: A text book of Quantitative inorganic Analysis , Lonqmans.
- 7) G. H. Morrison and H, Freiser : Solvent Extraction in Analytical Chemistry (John Wiley New
- 8) York, 1958)
- 9) Willard, Merrit and Settle : Instrumental Methods of analysis.
- 10) Principles of instrumental analysis- Holler, Skoog and Crouch
- 11) Instrumental methods of Chemical analysis-H. Kaur
- 12) Bhushan, Bharat 2004. Handbook of Nanotechnology. Springer.
- 13) Niemeyer, C.M. & Mirkin, C.A. 2004. Nanobiotechnology- Concepts, Applications and
- 14) Prespectives. Wiley-VCH Verlag.
- 15) Zander, C., Enderlein, J. & Keller, R.A. 2002 Single Molecule Detection in Solution. Wiley-VCH Verlag.
- 16) Avouris, P, Klitzing, K. Von, Sakaki, H. & Wiesendanger, R. 2003 NanoScience and Technology
- 17) Series. Scanning Probe Microscopy- Analytical Methods (R. Wiesendanger eds), Springer.
- 18) Instrumental Analysis by Skoog
- 19) Nanochemistry, a chemical approach to nanomaterials, G. A. Ozin, and A. C. Arsenault, RSC Publishing, Cambridge, 2005. ISBN 0-85404-664-X.

#### Paper No. -X, ACH 3.2: ORGANO ANALYTICAL CHEMISTRY

#### **UNIT–I: Hyphenated Techniques**

Advanced techniques of analysis: UV-Visible, IR, 1H-NMR (Recapitulation), 13CNMR, Mass spectrometry (Basic fundamentals of mass spectrometry, ionization, advanced organic analysis examples); Problems related to structure determination and applications of spectroscopic techniques as analytical tools.

#### **UNIT-II : A) Drug Analysis**

Introduction to drugs, their classification, sources of impurities in pharmaceutical raw materials such as chemical, atmospheric and microbial contaminants etc. Limit tests: Limit test for impurities for Pb, As, Fe, Se, etc. Estimation of moisture (K-F method), halide (Schnoiger's oxygen flask method), sulfate, boron, etc. Analysis of commonly used drugs such as antihistamines, sulfa drugs, barbiturates, etc. using non-aqueous titrations, sodium nitrite titrations, differential UV methods, colorimetric and fluorimetric methods of analysis.

#### **B)** Analysis of vitamins

Analysis of vitamins (thiamine, ascorbic acid, Vit. A, Vit. B6, Vit. K) and hormones (progesterone, oxytocin, insulin) chemical, instrumental and biological assay, wherever applicable.

#### UNIT – III: A) Clinical Analysis

Biological significance, analysis of assay of enzymes (pepsin, monoamine, oxidase, tyrosinase), Composition and detection of abnormal level of certain constituents leading to diagnosis of

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diseases. Sample collection and preservation of physiological fluids, analytical methods to the constituents of physiological fluids (blood, urine and serum). Blood- Estimation of glucose, chlolesterol, urea, hemoglobin and bilirubin, Urine- urea, uric acid, creatinine, calcium, phosphate, sodium, potassium and chloride.

#### **B)** Body fluid analysis

Composition and detection of abnormal level of certain constituents leading to diagnosis of diseases. Sample collection and preservation of physiological fluids, analytical methods to the constituents of physiological fluids (blood, urine and serum) Blood-Estimation of glucose, chlolesterol, urea, hemoglobin and bilirubin Urine- urea, uric acid, creatinine, calcium, phosphate, sodium, potassium and chloride.

#### **UNIT-IV: A)** Pesticides Analysis

Introduction, classification of pesticides, sampling, sample pretreatment and processin g, analysis of DDT, gammexane, endosulphan, zinab, ziram, malathion, thiram, thiometon, simazine and chloridane. Applications of colorimetric and chromatographic techniques (GC-MS, HPLC-MS) in analysis of pesticide residue. Introduction to EPA regulatory body. Practical applications and examples in analytical chemistry and research.

#### **B)** Forensic Analysis

Special features of forensic analysis, sampling, sample storage, sample dissolution, classification of poisons, lethal dose, significance of LD-50 and LC-50. General discussion of poisons with special reference to mode of action of cyanide, organophosphate and snake venom. Estimation of poisonous materials such as lead, mercury and arsenic in biological samples. Practical applications and examples in analytical chemistry and research.

#### **Reference Books:**

- 1) F. J. Welcher: Standard methods of Chemical analysis, 6th Ed. Vol. I and II( D. Van Nostard Comp.)
- 2) I. M. Kolthoff: Treatise on Analytical Chemistry Vol. I & II
- 3) F. D. Snell: Encyclopedia of industrial Chemical Analysis Vol. 1 to 20 ( John Wiley)
- 4) Riech: Outline of Indutrial Chemistry.
- 5) K. H. Buchel: Chemistry of Pesticides (John Wiley)
- 6) Indian, Pharmacopoeia, British Pharmacopoeia and U. S. Pharmacopoeia.
- 7) V. M. Parikh: Absorption spectroscopy of organic molecules (Addision Wesley)
- 8) Willard, Merrite, Dean and Settle: Instrumental methods of analysis (CBS)
- 9) D. H. Williams and J. Fleming: Specroscopic methods in organic chemistry (Mc Graw Hill)
- 10) Silverstein : Spectroscopic Identification of organic compounds (John Wiley)
- 11) Jackmann and Sternhill : Applications of NMR spectroscopy of organic Chemistry (Pergamon Press)
- 12) J. D. Roberts : Nuclear Magnetic Resonance (Mc Graw Hill)
- 13) K. Benjamin : Mass Spectrometry
- 14) Nichollas: Aids to the Analysis of foods and Drugs.
- 15) A. H. Beckett and J. B. Stanlake; Practical Pharmaceutical Chemistry Vol. I & II (CBS publishers)

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- 16) S. Ranganna:Handbook of analysis and quality control for fruits and vegetable products (McGraw Hill)
- 17) Ramalu: Analysis of pesticides

#### Paper No. -XI, ACH 3.3: ELECTROANALYTICAL TECHNIQUES IN CHEMICAL ANALYSIS

#### **UNIT-I: Voltammetry Techniques**

Introduction, Principle, excitation signals in voltammetry, basic instrumentation based on operational amplifiers, voltammetric electrodes

Cyclic Voltammetry: Instrumentation, Determination of analytes using cyclicvoltammetry, Applications. Pulse voltammetry: Introduction, Normal Pulse Voltammetry, Reverse pulse voltammetry, Differential pulse voltammetry, Square wave voltammetry. Stripping voltammetry: Cathodic and Anodic stripping voltammetry, Electrodeposition step, Voltammetric completion of the analysis, adsorptive striping methods, voltammetry with microelectrodes. Practical applications in analytical chemistry and research.

#### **UNIT- II: Colloids and emulsion**

**Colloids**: Colloidal solution, classification of colloids, Theories of origin of charge on sol particles, Determination of charge on a colloidal particle, Stability of sols, Association colloids, Spontaneous ageing of colloids, Factors affecting the spontaneous ageing, theories of spontaneous ageing, coagulation, kinetics of coagulation. Practical applications in analytical chemistry and research.

**Emulsion:** Types of emulsion, preparation, properties, Characteristics, Identification test between two types of emulsions, emulsifiers, demulsification. Gels: classification, methods for the preparation of gels, properties of gels, Applications of colloid science. Practical applications in analytical chemistry and research.

#### **UNIT –III: Particle Size Analysis**

Introduction, Low angle LASER light scattering: Instrumentation, theoretical models, Mie theory, Fraunhofer diffraction theory, particle size distribution analysis, Applications. Dynamic Light Scattering: Introduction, Instrumentation, photodetector sample cell and sample handling, Applications, Photosedimentation: Setting velocity and particle size, Stokes equation, Instrumentation, sedimentation modes, Particle size distribution analysis, photometric measurements and applications. Comparison with particle size measurements using XRD, SEM and TEM. Practical applications in analytical chemistry and research.

#### UNIT –IV: A) Ion selective electrodes

Terminology, types and construction of electrodes, glass electrode, solid state and precipitate electrodes, liquid – liquid membrane electrodes, enzyme and gas electrodes, and applications. B) Electrophoresis (05)

Introduction: paper electrophoresis: Technique, factors affecting migration of ions, capillary and zone electrophoresis and applications. Practical applications in analytical chemistry and research

#### **Reference Books:**

- 1) R.D. Braun, Introduction to Instrumental Analysis.
- 2) D.A.Skoog, F. J. Holler, Principles of Instrumental Analysis, 6th edition.

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- 3) Willard, Deritt, Dean and Settle, Instrumental methods of Analysis.
- 4) F. J. Welcher, Standard Methods of chemical Analysis Vol.3, PartA & B.
- 5) G.W. Ewing, Instrumental Methods of Analysis 4th and 5th editions.
- 6) Chatawal and Anand, Instrumental Methods of Analysis.
- 7) Bassett, Denney-Jeffer and Mendham, Vogel's Textbook of Quantitative Inorganic Analysis,(5th edition).
- 8) Electro-analytical chemistry, edited by H.W. Nurnberg.
- 9) Stulic, Ion selective electrodes (John Wiley).

#### **ELECTIVE PAPERS**

# Paper No. –XII(A), ACH 3.4(A): ENVIRONMENTAL CHEMICAL ANALYSIS AND CONTROL

#### **UNIT-I:** Sampling in analysis

Definition, theory and techniques of sampling, sampling of gas, liquids and solids, Criteria of Good sampling, Minimization of Variables, transmission and storage of samples, high pressure ashing techniques (HPAT), particulate matter, its separation in gas stream, Filtering and gravity separation. Analysis of particulate matter like asbestos, mica, dust and aerosols etc

#### UNIT-II: Electrochemical and spectral methods Environmental analysis (15)

Introduction to instrumental techniques, principle instrumentation and applications with respect to environmental analysis of Conductometry, Potentiometry, Ion selective electrodes, Cyclic voltammetry, Amperometry, Coulometry, Atomic absorption spectrometry, Atomic fluorescence spectrometry, Inductively coupled plasma spectrometry, Turbidimetry, Non Dispersive Infrared Analysis (NDIR).

#### **UNIT-III: Air and Water Pollutant Analysis**

Chemistry of Air pollutants, characterization. source, methods of analysis of air pollutants; CO,  $CO_2$ ,  $NO_X$ ,  $NH_3$ ,  $H_2S$ ,  $SO_2$  etc. Monitoring Instruments, Potable and Industrial water, major and minor components, dissolved oxygen (DO) Chemical oxygen demand(COD) Biochemical oxygen demand (BOD) and their measurements. Analysis of Pd, Cd, Hg, Cr, As and their physiological manifestations. Quality of industrial water analysis for organic and inorganic constituents. Chemistry of odour and its measurements.

#### **UNIT-IV: Organic Pollutants and Their Analysis**

Sources, disposal, treatment and analysis of phenolic residues, methods of recovery of phenols from liquid effluents, Organomercurials and its analysis, Analysis of organochlorine pesticides, volatile organic pollutants and their analysis

#### **Recommended books:**

- 1) A.K. De : Standard Methods of Waste and Waste water analysis.
- 2) P. M. S. Monk Fundamentals of Electroanalytical chemistry-John Wiley & Sons (2001) 3. Instrumental methods of chemical analysis H. Kaur
- 3) S.M. Khopkar, Environmental Chemistry; Environmental pollution analysis
- 4) M.S. Creos and Morr, Environmental Chemical Analysis, American publication(1988)

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- 5) A.K. De, Environmental Chemistry, New Age International publishers.Moghe and Ramteke, Water and waste water analysis : (NEERI)
- 6) A.C. Stern, Air pollution: Engineering control Vol.IV(AP)
- 7) P.N.Cheremisinoff and R.A.Young, Air Pollution controland Design.Hand Book Vol.I&II (Dekker)
- 8) R.B.Pohasek, Toxic and Hazardous waste disposal, Vol.I & II (AAS)
- 9) M.Sitting, Resources Recovery and Recycling, Handbook of industrial Waste.
- 10) B.K.Sharma, Industrial Chemistry.
- 11) S.P.Mahajan, Pollution Control in Process Industries.
- 12) R.A.Horne, Chemistry of our Environment.

#### Paper No. - XII(B), ACH 3.4(B): RECENT ADVANCES IN ANALYTICAL CHEMISTRY

#### UNIT-I: Ultra Purity and Ultra trace Analysis

Ultra purity and ultra trace analysis, laboratory dosing, purification of reagents, Preconcentration Techniques, Methods of trace analysis such as NAA, XRF, AAS and ICP, High purity materials for electronic industry, contamination control during analytical operations.

#### **UNIT-II: Radio-analytical Chemistry**

Separation methods, Precipitation, solvent extraction and chromatographic methods. Activation analysis, basic principles, fast neutron activation analysis, radiochemical methods in activation analysis, Applications if Geo-chemistry, oxygen in metals. Isotope dilution analysis: Principles and applications. Sub-stoichiometric determination of traces of metals: Principles, techniques and experimental methods in the determination of As, Pb and Hg.

#### **UNITS-III: Advanced Techniques in Analysis**

 $C^{13}$ ,  $P^{15}$  and  $O^{17}$  NMR Spectroscopy applications.

#### **UNIT-IV: Electron Spin Resonance Spectroscopy**

Electron behavior, ESR spectrometer, Spectra, Hyperfine interaction, free radical and interpretation of the spectra, Applications in quantitative analysis. Numerical problems.

#### Reference

- 1) Garen W. Ewing, Analytical Instrumentation, Handbook, Marcel Dekker Inc. (1997).
- 2) Mereitt, Dean, Settel, Instrumental methods of Chemical Analysis.
- 3) M. Zeif and J.W.Mitchell, Contamination Control in trace elemental analysis.
- 4) Ajuja, Ultrapurity.
- 5) Minczewski, Chwastowska and Dycozynski, Separation and pre-concentration methods in Inorganic trace analysis. Ellis Haward.
- 6) Cali, trace Analysis of semiconductor Materials Pergamon.
- 7) Overman and Cleark, Radioisotopes techniques MGH.
- 8) Tolgyessy, Brown and Kyrs, Isotope dilution analysis.
- 9) Leniham and Thomson, Activation Analysis(AP)
- 10) Ruzica and Stary, Substopchiometry in Radiochemical Analysis. Pergamon.
- 11) Ladd and Lee, Radiochemistry.
- 12) Clerk, Handbook of Radiochemical methods
- 13) Price, Nuclear radiation detections.

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# Paper No. – XII(C), ACH 3.4(C) : CHEMICAL ANALYSIS IN AGRO, FOOD AND PHARMACEUTICAL INDUSTRIES.

#### UNIT – I: Analysis of soil, Fuel, Body Fluids and Drugs

Analysis of soil: Moister, pH, total nitrogen, phosphorous, silica, lime, Magnesia, Manganese, sulfur & alkali salts. Food analysis: Solid, liquid and Gas, ultimate and proximate analysis heating values , grading of cool, liquid fuels, flasks points, aniline point, octane number and carbon residue, gaseous fuels – producer gas and water gas – calorific value.

#### **UNIT-II: Clinical Chemistry**

Composition of blood collection, and preparation of samples, clinical analysis – serum electrolytes, blood glucose, blood urea nitrogen , uric acid , albumin , globulin , barbiturates , acidic and alkaline phosphates, Immunoassay , principals of radioimmunoassay, and applications . The blood gas analysis– trace elements in the body. Drug analysis: Narcotics and dangerous drugs, classification of drugs, screening by gas m thin layer chromatography and spectrophotometric analysis.

#### **UNIT – III: Food analysis**

Moister, ash, crude protein, fat, crud fiber, carbohydrate, calcium, potassium, sodium, and phosphates, food adulteration – common adulteration in food, contamination of food stuffs, microscopic examination of foods for adulterants, Pesticide analysis in food products, Bxdraction and purification of sample, HPLC, gas chromatography for organo – phosphates, thin layer chromatography for identification of chlorinated pesticides in food products

### UNIT –IV: Fluorescence in Biological, Medical and Drug Development (15)

Fluorescence instrumentation for analysis, fluro phare and their modification, pH-indicators, membrane potential probes, lipid membrane protein labeling of protein and DNA.

#### References

- 1) Fundamentals of Analytical Chemistry by D. A. Skoog, D. M. West and F. J. Honer, W. B. Saunders.
- 2) Chromic phenomenon, The Technological application of color chemistry Peter Bamfield. Practical Course

# M.Sc. Part-II (Sem-III)

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# Analytical Chemistry Practical Course ACHP-V and ACHP-VI List of Experiments:

#### Major:

- 1. Estimation of Sn, Zn, Cu and Pb from Bronze alloy (volumetric, gravimetric or colorimetric techniques can be used)
- 2. Estimation of Ca and Fe from milk powder
- 3. Analysis of Galena ore
- 4. Analysis of Benzoic acid and salicylic acid from medicated powder
- 5. Analysis of vitamin A in food products
- 6. Estimation of Aspirin
- 7. Kjeldahl's method of protein estimation in foods and feeds
- 8. Analysis of Lindane in BHC powder.
- 9. Determination of pK value of an indicator.
- 10. Polarographic estimation of traces of Cu, Cd, Ni, Zn and Fe in sample solution.
- 11. To study the complex formation between Fe(III) and salicylic acid and determine the stability constants of the complex by Job's variation method.
- 12. To determine the equivalence conductance and dissociation constant using Kolharach Law at infinite dilution independent of ionic mobility of weak electrolyte.
- 13. Any other suitable experiment may be added when required.

### Minor:

- 1. Analysis of plaster of Paris for calcium content
- 2. Fertilizer analysis for P (colorimetrically), K (Flame photometrically).
- 3. Determination of Barium ions by Turbidimetry.
- 4. Analysis of iodized table salt.
- 5. Analysis of soda ash.
- 6. Estimation of copper fungicide
- 7. Analysis of sulpha drug
- 8. Analysis of vitamin-C in juices and squashes.
- 9. Analysis of ethambutol
- 10. Identification of organic compounds by their IR spectra
- 11. Determination of strength of acetic acid in commercial vinegar by conductometric method.
- 12. Determination of chloride content from saline water by potentiometry.
- 13. Estimation of bicarbonate and carbonate by potentiometric method.
- 14. Estimation of Fe by ceric sulphate and potassium dichromate titration potentiometrically.
- 15. XRD and Thermal analysis Kaolinite, cobalt oxalate and zinc oxalate.
- 16. Estimation of vitamin B2 in the medicinal tablets fluorimetrically.
- 17. Kinetic study of hydrolysis of ethyl acetate in presence of OH ions conductometrically.
- 18. Determination of pK of given dibasic acid pH-metrically.
- 19. Determination of relative strength of acetic acid, chloroacetic acid and trichloro acetic acid by conductometrically.
  - (At least 10 major and 10 minor experiments should be carried out)

# M.Sc. Part-II (Sem-IV) Analytical Chemistry

#### Paper No. -XIII, ACH 4.1: MODERN SEPARATION METHODS IN ANALYSIS

#### **UNIT-I: Advanced Gas Chromatographic Techniques**

Principles, Plate theory, Instrumentation and working of a Gas Chromatograph, sampling, sample pretreatment, sample injection types, columns, Detectors, programmed temperature G.C., Applications. Pyrolysis gas and vapour phase chromatography-instrumentation and techniques, advantages and applications. Gas chromatography-Mass Spectrometry, interface, instrumentation and applications. Introduction to TGA-MS/TGA-GC-MS and significance. Practical applications and examples in analytical chemistry and research.

#### **UNIT-II: Advanced Liquid Chromatographic Techniques**

High Performance Liquid Chromatography (HPLC) and Ultra Performance Liquid Chromatography (UPLC)-Principle, instrumentation, mobile phase, Stationary support in HPLC, detectors and applications. Super critical fluid chromatography (SCFC), characteristics, instrumentation and applications. Comparison of HPLC and GLC with SCFC. Liquid Chromatography-Mass Spectrometry interface, instrumentation, advantages and applications. Practical applications and examples in analytical chemistry and research.

#### **UNIT-III: Ion Chromatography**

Principles, structure and characteristics of resins, eluent, supressor columns and detectors used in Ion Chromatography, commercial scope, analytical applications, environmental speciation by Ion Chromatography. Practical applications and examples in analytical chemistry and research.

#### UNIT –IV: A) Modern extraction and separation techniques

Basic principles, classification of solvents extraction systems, extraction equilibria, factors affecting extraction process, application of  $\beta$ - diketones,  $\delta$ Hydroxyquinoline, dithicarbamaes, xanthenes, Thio, separation of non metals and metals. Separation of transition metal ions using ion exchangers.

Solid phase extraction, solid phase microextraction, sonic extraction, accelerated solvent extraction, soxhlet extraction.

#### B) Extractive Chromatographic Separations

Introduction, Theoretical aspects of extraction chromatography, solvent extraction and extraction chromatography with chelating ligands, extraction chromatography by ion pair formation, extraction chromatography by solvation, extraction equilibria, nature of stationary phase in extraction chromatography, inert support, techniques in extraction chromatography, extraction chromatography with tributyl phosphate and other applications. Practical applications and examples in analytical chemistry and research.

#### **Recommended Books:**

- 1) A.I.Vogel, a text Book of Quantitative Inorganic Analysis.
- 2) W H Willard, L L Merritt and J A Dean, Instrumental Methods of Analysis.
- 3) S. M.Khopkar, Basic Concepts in Analytical Chemistry.
- 4) LR. Shyder and C.H.Harvath, An Introduction to separation Science. Wiley Interscience.
- 5) James S Fritz and George H.Schenk Jr. Quantitative Analytical Chemistry, 2nd editions Allyn and Bacon Inc. Bosten.
- 6) J.G.Dick, Analytical Chemistry.
- 7) R.L.Pescok and L.D.Shield, Modern Methods of Chemical Analysis.
- 8) O.Samuelson : Ion Exchange separation in analytical chemistry (Jhonwiley, 1963)

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- 9) Y. Marcus and A. S. Kertes : Ion Exchange and solvent Extraction of metal complexes (Wiley – Interscience, 1969)
- 10) J. A. Marinsky and Y. Marcus : Ion exchange and solvent Extraction (Marcel Dekker, INC, New York, 1973)
- 11) G. H. Morrison and H, Freiser : Solvent Extraction in Analytical Chemistry (John Wiley, New York, 1958)
- 12) A. K. Da, S. M. Khopkar and R. A. chalmers :solvents Extraction of metals (Von Nostrant Ravinhold, 1970)

#### Paper No. -XIV, ACH 4.2: ORGANIC INDUSTRIAL ANALYSIS

#### **UNIT – I: Industrial Analysis**

#### A) Analysis of oils, fats and Soaps

Introduction to natural fats and oils; isolation of oils from natural resources and their purification. Analysis of oils and fats: Softening point, Congeal point, Titre point, Cloud point, Iodine, saponification, acid, hyroxyl, R-M and Polenske value, Elaiden test, etc.

Introduction to soaps, manufacture of soaps (in brief), analysis of soaps: total anhydrous soap and combined alkali, potassium, water, free fatty acids, saponifiable and non-saponifiable matter in soaps, estimation of phenol, copper and germicidal agents in soaps, determination of inorganic fillers and soap builders, and other additives, estimation of soap in detergents (THAM method)

#### **B)** Analysis of Detergents

Classification of detergents, analysis of raw materials, separation as alcohol soluble and alcohol insoluble matter, additives in detergent formulation (chlorides, sulfates, phosphates, silicates, borates, oxygen releasing substances, CMC, EDTA, etc.), their role and analysis; analysis of active ingredients in detergents (methylene blue and Hyamine-1622 method).

#### **UNIT - II: Food and Food Additive Analysis**

#### A) Food Analysis

Food flavors, food colors, food preservatives, analysis of milk and milk products, adulterants in milk and their identification, analysis of honey, jam and their major component. Practical applications and examples in analytical chemistry and research.

#### **Food Additive Analysis** B)

Additives in animal food stuff: Antibiotics: penicillin, chlorotetracyclin, oxytetracyclin in diet supplements; Identification and estimation of growth promoting drugs such as. sulfaquinoxaline, methyl benzoquate, sulfanitran, pyrimethamine, nitrovin, nitrofurazone, acinitrazole, etc

#### **UNIT-III: Analysis of cosmetics products**

Introduction to cosmetics, definition, types of cosmetics, background, development in cosmetic industry, issues in cosmetic industries (contamination and adulteration), future scope and role of analytical chemistry.

#### A) Analysis of cream and lotions

Composition of creams and lotions, determination of water, propylene glycol, non-volatile matter and ash content; estimation of borates, carbonates, sulphates, phosphates, chlorides,

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Composition of face powder, estimation of boric acid, Mg, Ca, Zn, Fe, Al and Ba. Analysis of deodorants and antiperspirants-composition, analysis of fats and fatty acids, boric acid, magnesium, calcium, zinc, iron, titanium, aluminium, phenol, methanamine, hexachlorophenone, sulphonates, urea, etc. Practical applications and examples in analytical chemistry and research.

ammonia, nitromethane, oxalic acid, 4- hydroxy benzoic acid, sodium iodate, free formaldehyde, H2O2, mercatoacetic acid, titanium and zinc oxides. Practical applications and

#### UNIT-IV: Analysis of Paints, pigments and petroleum products

#### A) Analysis of Paints and pigments

**B)** Analysis of face powder

examples in analytical chemistry and research.

Composition of paint, preliminary inspection of sample, test on the total coating, separation and estimation of pigments, binder and thinner of latex paints; modification of binder, flash point of paints. Practical applications and examples in analytical chemistry and research.

#### (B)Analysis of petroleum products

Introduction, constituents and petroleum fractionation, quality control; - specific gravity, viscosity, Cloud point, pour point, flash point, vapor pressure, Doctor test, sulphuric acid absorption, aniline point, and colour détermination, cloud point, pour point. Determination of water, neutralization value (acid and base numbers), ash content, sulphur and mercaptan sulphur. Determination of lead in petroleum; Analysis of coal and coke: Types, composition, preparation of sample, proximate and ultimate analysis calorific value by Bomb Colorimetry.

#### **Reference Books:**

- 1) S. R. Junk and H. M. Pancoast: Hand book of sugars(AVI)
- 2) B. Bilot and B. V. Well: Perfumary technology (JW)
- 3) I. M. Kolthoff: Treatise on Analytical Chemistry Vol. I and II
- 4) D. Pearson: Laboratory techniques in food analysis.
- 5) S. Ranganna: Handbook of Analysis and Quality control for fruits and vegetable products, 2nd Ed.(Mc Graw Hill.)
- 6) Nicholls : Aids to the analysis of foods and drugs.
- 7) G. J. Mountrey: Poultry product technology (AVI)
- 8) Karamer Twig: Quality control for food industry (AVI)
- 9) G. F. Longonan: the analysis of detergents and detergent products (JW)
- 10) A. Davidsohn & B. M. Mlwidaky : Synthetic detergents (Book center, Mumbai)
- 11) M. Ash and L. Ash: A formulary of cosmetic preparations. (G. Goodwin)
- 12) Kurl Bauer, Dorothea Garhe, Horst Surburg: Common fregrance and flavour materials, (VCH publisher, New York)
- 13) F. J. Welcher: Standard Methods of Chemical analysis Vol I & II (6th Ed.)
- 14) S. N. Mahendru: Analysis of food products (Swan Publishers)

#### Paper No. - XV, ACH 4.3: ADVANCED METHODS IN CHEMICAL ANALYSIS

#### **UNIT-I : Fluorescence and Phosphorescence Spectrophotometry**

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Fluorimetry, types of luminescence, Instrumentations, theories of fluorescence and phosphorescence, electronic transition, structural factors, solvatochromism, solvation dynamics, faith of excited molecules, solvent effect on fluorescence, effect of intermolecular process,

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fluorescence anisotropy and time domain fluorescence life time measurements. Relation between concentration with fluorescence and phosphorescence intensity, fluorescence quenching mechanism, resonance energy transfer. Chemiluminescence, Fluorescence sensing, Synchronous spectrum, Fluorescent nanomaterials. Practical applications, examples and problems in analytical chemistry and research.

#### **UNIT-II: Kinetic Methods**

Theoretical basis of kinetic methods of analysis, methods of determining amount of the substance, Tangent Method, Fixed Time and Concentration method. Addition Method, Oxidation Reactions of H2O2 with thiosulphate, iodide and amino, Enzyme catalyzed reactions. Inhibitors and Activators.

#### **UNIT – III: Photoelectron spectroscopy**

Basic principles, photoelectric effects, Photoionization process, Koopman's theorem, photoelectron spectra of simple molecules, ESCA, chemical shift, Auger electron spectroscopy – basic idea.

#### **UNIT-IV: X-ray spectroscopy**

Introduction, X-Ray generation, Properties of X-radiation, X-Ray, Instrumentation, X-Ray Absorption, Fluorescence and Diffraction methods of analysis and their applications

#### **Recommended Books:**

- 1) Gary D Christian, Analytical chemistry 6<sup>th</sup> edition. John Willey and sons INC (2003) H.
- 2) Kaur, Instrumental Methods of Chemical Analysis. Pragati Prakashan, Meerut.
- 3) W H Willard, L L Merritt and J A Dean, Instrumental Methods of Analysis.
- 4) S. M.Khopkar, Basic Concepts in Analytical Chemistry.
- 5) D. Skoog and D. West, Principle of Instrumental Analysis.Holl Seamlers.
- 6) E. Berlin, Principles and Practice of X-Ray Spectrometric Analysis, Plenum, NewYork.
- 7) J. Winefordner, S. Schulman and T O Haver :Luminescence Spectrometry in
- 8) Analytical Chemistry. Wiely Interscience NewYork.
- 9) H. Mark and G Rachnitz, Kinetics in Analytical chemistry. Interscience NY.
- 10) 8.Gary D Christian, Analytical chemistry 6<sup>th</sup> edition. John Willey and sons INC (2003)
- 11) Engineering chemistry, R Gopalan, G. S. Nagrajan.
- 12) 10 Engineering chemistry B. K. Sharma

#### **ELECTIVE PAPERS**

#### Paper No. -XVI(A), ACH 4.4(A): APPLIED ANALYTICAL CHEMISTRY

#### **UNIT-I: Spectrochemical Methods of Analysis**

Introduction to spectrochemical methods. Electronic spectra and molecular structure, NIR spectrometry for nondestructive testing. Solvents for spectrometry ,FTIR spectrometer ,fluorometry, optical sensors. Analysis of ores –bauxites, dolomites, monazites. Analysis of Portland cement.

#### **UNIT-II: Analysis of metals and alloys**

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Foundry materials, ferroalloys, and special steels, slags, fluxes. Analysis of alloys ,bronze, brass, Alnico and Nichrom

#### UNIT-III: Analysis of soil and fertilizers

Method of soil analysis, soil fertility its determination, determination of inorganic constituents of plant materials, Chemical analysis as measure of soil fertility, analysis of fertilizers.

#### **UNIT-IV: Analysis of Commercial materials**

Analysis of explosive materials, TNT, RDX, lead azide, EDNA (ethylene dinitramine). Analysis of conducting polymer, resins and rubber. Analysis of luminescent paints, Analysis of lubricants and adhesive.

#### **Recommended Books:**

- 1) Hillebrand Lhundel, Bright and Hoffiman, Applied Inorganic Analysis, John Wiley.
- 2) Snell and Biffen, Commercial Methods of Analysis.
- 3) P.G. Jeffery, Chemical Methods of Rock Analysis, Pergamon.
- 4) Buchel, Chemistry of Pesticides. J Wiley.
- 5) Rieche, Outlines of Industrial Organic Chemistry, ButterWorth.
- 6) F.A.Henglein, Chemical Technology, Pergamon.
- 7) Kent, Riegl's Industrial Chemistry, Rainhold.
- 8) Chopra and Kanwar, Analytical Agriculture Chemistry, Kalyani Publishers.
- 9) Aubert and Pintes, Trace Elements in Soils.
- 10) Bear, Chemistry of Soil.
- 11) Hauson, Plant Growth Regulators, Noyes.
- 12) P.G.Jeffery and D.J. Hatchinson, Chemical Methods of Rock Analysis.
- 13) F.J.Weleher, Standard Methods of Chemical Analysis, A Series of Volumes Robert and Krigeger Publishing Company.
- 14) I. M.Kolthoff and PJ Ewing, Treatise o Analytical Chemistry, A series of Volumes.
- 15) R.D. Reeves and R.R. Brooks, Trace element Analysisof Geological Materials, John Wiley & Sons NewDehli.
- 16) W.M. Johnson and J.A.Maxwell,Rock and Mineral Analysis, John Wiley and Sons, NewYork.
- 17) W. F. Hildebrand, G H C Landell and HABrighot, Applied Inorganic Analysis, John Wiley 2nd Edition.
- 18) K. J. Das, Pesticide Analysis(MD).

#### Paper No. -XVI(B), ACH 4.4(B): QUALITY ASSURANCE AND ACCREDITATION

#### **UNIT-I: Quality Assurance**

Introduction to Quality Control and quality assurance: Concepts and significance. Quality control and statistical techniques: Quality control charts, the X-quality control chart, the R-quality control chart and its interpretation, spiked sample control charts, use of blind samples in quality control, use of proficiency evaluations in quality control. Calibration and maintenance of Instruments / Equipment: Instrument calibration – linear calibration curves, equipment calibration, frequency of calibration, calibration of common laboratory instrument and equipment (Analytical balances, volumetric glassware, ovens, furnaces, UV / Visible spectrophotometer, pH meter, conductivity meter, IR spectrophotometers, AAS, GC, HPLC etc.,). Maintenance of instruments and equipment

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#### **UNIT-II: Documentation for Quality Assurance: Raw Data**

Type of notebooks, control of notebook distribution and data entry. General Reagents and volumetric reagents. Sampling - sampling methods, sample labelling, sample login/register. Sample analysis, reporting, recording and personal training.Instrument calibration and maintenance. Analytical report, Personnel, training, records - professional personnel, technician personnel. Filing quality assurance documentation. Good laboratory practices and personnel, Quality Programme, Instrument and Organisation calibration, Customer Satisfaction.

#### **UNIT-III: Documentation for Quality Assurance: Raw Data**

(15)Computers and quality assurance: Sample handling. Data Acquisition. Quality control data and calculations. Computer generated analytical reports. Security considerations. Hardware and software. Establishing a Quality Assurance program: Management commitment. Define the quality assurance program. Writing standard operating procedures. Topics for standard operating procedures. Consolidating the programme. Monitoring the program - monitoring quality assurance data, reporting quality assurance problems. Writing the quality assurance manuals. (15)

#### **UNIT-IV** Quality Accreditation

Laboratory Accreditation: Need for laboratory accreditation. International aspects of laboratory accreditation and in India. Criteria for laboratory accreditation. Benefits of laboratory accreditation, Evolution and significance of Quality Management, Background to ISO 9000, comparison between ISO-9001, ISO-9002 & ISO-9003., ISO 9000-2000 series of standards on quality managament system,- evolution of series of standards, introduction to ISO organization, Registration/ certification- benefits of QMS certification. Structure of ISO 9000-2000 family of standards. Advantages of ISO 9000-2000. Requirements of ISO 9001-2000 QMS and applications, Steps for effective implementations. Significance of ISO - 9001, 9002, 9003 & 9004. Requirements of ISO9000/ IS14001. Concepts of OHSMS (BS 8800) Quality Managament Principles in OMS, OMS documentation, Quality Manual, Quality policy, conformities and Nonconformities

#### **Recommended Books:**

- 1) Handbook of Quality Assurance for the analytical chemistry laboratory, James P. Dux, Van Nostrand Reinhold, New York, 1986.
- 2) Applying ISO-9000 Quality Management Systems, International Trade Centre Publishing, UNCTAD/WTO. Geneva, Switzerland, Indian Edition Printed by D.L.Shah Trust.
- 3) How to practice GLP, PP Sharma, Vandana Publications, 2000, New Delhi
- 4) Training manuals on ISO 9000 / 2000 PQM, Girdhar J Gyani, Raj Publishing House, 2001
- 5) Quality Assurance in Analytical Chemistry, B.W. Wenclawiak, Springer, India, 2004.

#### Paper No. -XVI(C), ACH 4.4(C): FORENSIC SCIENCE AND MICROBIOLOGICAL ANALYSIS

#### **UNIT-I: Forensic Analysis**

Special features of Forensic analysis, sampling, sample storage, sample dissolution classification of poisons, Lethal dose, significance of LD 50 and LC 50.

#### **UNIT-II: Identification and Analysis in the suspects**

Poisonous elements viz As, Sb, Pb, Cr and Hg.

i)Insecticides Analysis of metals, Gun powder Residues, portland cement in Forensic samples.

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ii) Poisoning due to cyanide dioxines & asbestos.

iii) Physiological effects of natural poisons such as Col Chicine, Morphine, Hashish ,Nicotinoids.

iv) Health hazards and Remedial measures.

# **Unit III: Analytical Microbiology**

Morphological structure and characteristics nutrition and physiology classification of microorganisms, Taxonomy and nomenclature Nutritional requirements, Phathoseas and Spoilage organics Microscopy, Staining techniques, Aspatic Techniques, isolation and use of differential media, sterilization and disinfection.

# **UNIT-IV: Applied Microbiology**

(15)Air Microbiology with respect contamination control, Food Microbiology, Water microbiology, Industrial microbiology with respect to quality control.

# **Recommended Books:**

- 1) Allan Cury, Irvins Sunshine, Forensic Analysis, Academic Press Publications.
- 2) E.G.J.Clarics, Isolation and Identification of drugs, Pharmaceutical Press.
- 3) C.J.Creswell, C.A.Runquist and M.M.Campbell, Spectral Analysis of Organic
- 4) Compounds.
- 5) F.J.Welcher, Robert E, Standard Methods of Chemical Analysis, A series of volumes.
- 6) Hawk's Physiological Chemistry.
- 7) D.J.Holme and H. Pack, Analytical Biochemistry, Longman.
- 8) G. Keleti and W H Liederer, Hand book of micro methods for the biological science-VNR.
- 9) C H Collins, Microbiological Methods, Butterworths.

# M.Sc. Part-II (Sem-IV)

# Analytical Chemistry Practical Course ACHP-VII and ACHP-VIII **List of Experiments:**

# Maior

- Cement analysis 1.
- Analysis of Chrome steel alloy for Cr and Ni content 2.
- Analysis of bauxite ore to estimate the amount of silica, aluminium and iron. 3.
- Estimation of salicylic acid and zinc oxide from medicated powder 4.
- 5. Determination of saponification value and iodine value of oil
- Estimation of amount of copper (II) with EDTA spectrophotometrically. 6.
- Simultaneous spectrophotometric determination of Cr and Mn 7.
- Analysis of milk. 8.
- Analysis of some common pesticides, insecticides, plastics and detergents. 9.
- Estimation of Urea, Uric acid and creathinine in Urine. 10.
- Estimation of blood sugar, calcium and total nitrogen and non-protein nitrogen in blood. 11.
- 12. Studies on the effect of substituent at ortho position of benzoic acid on its equilibrium constant pH metrically.
- Agricultural analysis of soil sample, animal feeds, soil micronutrients, milk powder for Ca, 13. Fe and P content.

# Minor

1. Estimation of Fe from soil sample

- 2. Analysis of Na and K from soil sample
- 3. Determination of chemical oxygen demand of water sample (dye solution)
- 4. Estimation of lactose from milk sample
- 5. Determination of flash point of oil/fuel
- 6. To estimate the amount of glycine from amino acid
- 7. To determine the amount of alkali content of antacid tablet titrimetrically
- 8. Determination of dissociation constant of weak acid pH-metrically.
- 9. Estimation of Zn in the given solution fluorimetrically.
- 10. Determination of pK of tribasic acid, by potentiometry.
- 11. Determination of critical micelle concentration of given surfactants conductometrically
- 12. Estimation of acetyl salicylic acid in the given aspirin tablet by titrating against 0.1N alcoholic KOH potentiometrically.
- 13. To determine the acid base dissociation constant and isoelectric point of amino acid pH metrically
- 14. (Any other experiments may be added when required.)

(At least 6 major and 6 minor experiments should be carried out. More time should be given to project work)

### **B) Project:**

Projects on contemporary issues of societal significance which should include literature survey, synthesis, reaction mechanism and kinetics, analysis of air, water and soil samples, solid state materials, energy generation and storage materials, nanochemistry, green chemistry, organic materials, organo-metallic, bioinorganic materials, novel materials etc. The Project/Review work (50 Marks) will be examined jointly by internal and external examiners at the time of practical examination.

(Any other experiments may be added when required.)

#### Study tour is compulsory for M.Sc. Part- II Students to visit Chemical Industries in India.

#### 15. Equivalence in Accordance with titles and contents of the papers

Old Course(2019)			New Course (2020)		
Paper No	Course Code	Title of the course	Paper No	Course Code	Title of the course
IX	ICH 3.1	Inorganic Chemical Spectroscopy	IX	ICH 3.1	Inorganic Chemical Spectroscopy
Х	ICH 3.2	Coordination Chemistry - I	X	ICH 3.2	Coordination Chemistry - I
XI	ICH 3.3	Nuclear Chemistry	XI	ICH 3.3	Nuclear Chemistry
XII(A)	ICH 3.4(A)	Organometallic and Bioinorganic Chemistry	XII(A)	ICH 3.4(A)	Organometallic and Bioinorganic Chemistry
XII(B)	ICH 3.4(B)	Selected Topics in Inorganic Chemistry	XII(B)	ICH 3.4(B)	Selected Topics in Inorganic Chemistry
XIII	ICH 4.1	Instrumental Techniques	XIII	ICH 4.1	Instrumental Techniques
XIV	ICH 4.2	Coordination Chemistry II	XIV	ICH 4.2	Coordination Chemistry II
XV	ICH 4.3	Chemistry of Inorganic Materials	XV	ICH 4.3	Chemistry of Inorganic Materials
XVI(A)	ICH 4.4(A)	Energy and Environmental Chemistry	XVI(A)	ICH 4.4(A)	Energy and Environmental Chemistry
XVI(B)	ICH 4.4(B)	Radiation Chemistry	XVI(B)	ICH 4.4(B)	Radiation Chemistry

# M. Sc. Part II (Semester III and IV) Inorganic Chemistry

# M. Sc. Part II ( Semester III and IV) Organic Chemistry

Old Course(2019)			New Course (2020)		
Paper No	Course Code	Title of the course	Paper No	Course Code	Title of the course
IX	OCH 3.1	Organic Reaction Mechanism	IX	OCH 3.1	Organic Reaction Mechanism
Х	OCH 3.2	Advanced Spectroscopic Methods	X	OCH 3.2	Advanced Spectroscopic Methods
XI	OCH 3.3	Advanced Synthetic Methods	XI	OCH 3.3	Advanced Synthetic Methods
XII(A)	OCH 3.4(A)	Drugs and Heterocycles	XII(A)	OCH 3.4(A)	Drugs and Heterocycles
XII(B)	OCH 3.4(B)	Polymer Chemistry	XII(B)	OCH 3.4(B)	Polymer Chemistry
XIII	OCH 4.1	Theoretical Organic Chemistry	XIII	OCH 4.1	Theoretical Organic Chemistry
XIV	OCH 4.2	Stereochemistry	XIV	OCH 4.2	Stereochemistry
XV	OCH 4.3	Chemistry of Natural Products	XV	OCH 4.3	Chemistry of Natural Products
XVI(A)	OCH 4.4(A)	Applied Organic Chemistry	XVI(A)	OCH 4.4(A)	Applied Organic Chemistry
XVI(B)	OCH 4.4(B)	Bioorganic Chemistry	XVI(B)	OCH 4.4(B)	Bioorganic Chemistry

Old Course(2019) New Course (2020)		e (2020)			
Paper No	Course	Title of the	Paper No	Course	Title of the
	Code	course		Code	course
IX	PCH 3.1	Advanced	IX	PCH 3.1	Advanced
		Quantum			Quantum
		Chemistry			Chemistry
Х	PCH 3.2	Electrochemistry	X	PCH 3.2	Electrochemistry
XI	PCH 3.3	Molecular	XI	PCH 3.3	Molecular
		Structure – I			Structure – I
XII(A)	PCH 3.4(A)	Solid State	XII(A)	PCH 3.4(A)	Solid State
		Chemistry			Chemistry
XII(B)	PCH 3.4(B)	Advanced	XII(B)	PCH 3.4(B)	Advanced
		Chemical			Chemical
		Kinetics			Kinetics
XII(C)	PCH 3.4(C)	Radiation and	XII(C)	PCH 3.4(C)	Radiation and
		Photochemistry			Photochemistry
XIII	PCH 4.1	Thermodynamics	XIII	PCH 4.1	Thermodynamics
		and Molecular			and Molecular
		Modeling			Modeling
XIV	PCH 4.2	Chemical	XIV	PCH 4.2	Chemical
		Kinetics			Kinetics
XV	PCH 4.3	Molecular	XV	PCH 4.3	Molecular
		Structure - II			Structure - II
XVI(A)	PCH 4.4(A)	Surface	XVI(A)	PCH 4.4(A)	Surface
		Chemistry			Chemistry
XVI(B)	PCH 4.4(B)	Chemistry of	XVI(B)	PCH 4.4(B)	Chemistry of
		Materials			Materials
XVI(C)	PCH 4.4(C)	Biophysical	XVI(C)	PCH 4.4(C)	Biophysical
		Chemistry			Chemistry

# M. Sc. Part II ( Semester III and IV) Analytical Chemistry

Old Course(2019)		New Course (2020)			
Paper No	Course Code	Title of the course	Paper No	Course Code	Title of the course
IX	ACH 3.1	Advanced Analytical Techniques	IX	ACH 3.1	Advanced Analytical Techniques
Х	ACH 3.2	Organo Analytical Chemistry	X	ACH 3.2	Organo Analytical Chemistry
XI	ACH 3.3	Electroanalytical Techniques in Chemical Analysis	XI	ACH 3.3	Electroanalytical Techniques in Chemical Analysis
XII(A)	ACH 3.4(A)	Environmental Chemical Analysis and Control	XII(A)	ACH 3.4(A)	Environmental Chemical Analysis and Control
XII(B)	ACH 3.4(B)	Recent Advances in Analytical Chemistry	XII(B)	ACH 3.4(B)	Recent Advances in Analytical Chemistry
XIII	ACH 4.1	Modern Separation Methods in Analysis	XIII	ACH 4.1	Modern Separation Methods in Analysis
XIV	ACH 4.2	Organic Industrial Analysis	XIV	ACH 4.2	Organic Industrial Analysis
XV	ACH 4.3	Advanced Methods in Chemical Analysis	XV	ACH 4.3	Advanced Methods in Chemical Analysis
XVI(A)	ACH 4.4(A)	Industrial Analytical Chemistry	XVI(A)	ACH 4.4(A)	Industrial Analytical Chemistry
XVI(B)	ACH 4.4(B)	Quality Assurance and Accreditation	XVI(B)	ACH 4.4(B)	Quality Assurance and Accreditation