

# Bundelkhand University, Jhansi

## Board of Studies

In accordance with NEP-2020

in accordance with NEP-2020

Name of Course			Subject			Faculty			Date of BOS 02/07/2022	
S.No	BOS member	Designation	Feed Back of Students	Revision of Syllabus (mentioned in percentage)	Credit Course	Non Credit Course	multidisciplinary Courses	Vocational/Skilled Orientation course	Number of value added course with title(Semester wise)	
1	Dr. Surabh Yadav.	convenor		20%	yes	—	yes	✓	✓	
2	Dr. M. Ajay Ansoni	Membr.								
3	Dr. Anil Kumar	Membr.								
4	Maya verma	Membr.								
5	Dr. Ekta Pandey	Expm Sulgy.								
6	Dr. Chitra Gupta	Co-ordi nator								
Comments										

Internal members 1 2

Dean

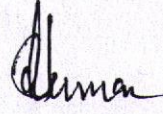
External Expert 1 External Expe

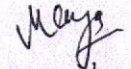


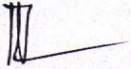
MASTER OF SCIENCE  
IN  
CHEMISTRY

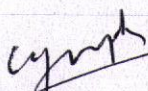
TWO YEARS FULL TIME PROGRAM.  
COURSE CONTENT OF  
VII, VIII, IX and X SEMESTER

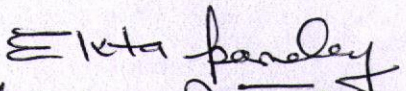
2022 JUNE

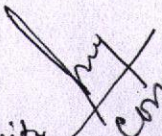
  
Dr. Anis Kumar  
Deptt. of  
Chemistry  
B.B.C.  
Jhansi

  
Dr. Mayaherna  
HOD  
Deptt. of Chemistry  
Govt. Girls PG College  
Banda

  
(Dr. M.A. Anand)

  
Dr. Chitra Singh  
(Co-ordinator)  
Deptt. of Chemistry  
Bundelkhand University  
V.P.)

  
(Dr. Elita Pandey)  
विषय विशेषज्ञ

  
convenor  
5/07/22



**Course Structure For M.Sc. Chemistry  
(VII-X Semester)**

SEME STER	PAPER CODE	PAPER	THEO RY (MAR KS-75 MAX.)	INTENRAL (MARKS -25)			CREDIT
			75	25*			
			75	10	10	5	
			75	10	10	5	
VII	CHY 701	Application of Computer in Chemistry	75				4
	CHY 702	Inorganic Chemistry	75				4
	CHY 703	Organic Chemistry	75				4
	CHY 704	Physical Chemistry	75				4
	CHY 705	Minor Elective Course	75				4
	CHY 706	Practical (Organic, Inorganic, & Physical Chemistry)	75				4
	CHY 707	Research Project/Industrial & field Training/ Survey	100	-	-	-	4
VIII	CHY 801	Inorganic and Group Theory	75				4
	CHY 802	Organic Chemistry	75				4
	CHY 803	Physical Chemistry	75				4
	CHY 804	Spectroscopy	75				4
	CHY 805	Practical (Inorganic, Organic, & Physical Chemistry)	75				4
	CHY 806	Research Project/Dissertation (continue 707)	100	-	-	-	4
IX	CHY 901	Application of spectroscopy	75				4
	CHY 902	Biochemistry	75				4
	CHY 9031-9034	Paper Elective	75				4
	CHY 9041-9044	Paper Elective	75				4
	CHY 905	Practical (Organic, Inorganic, & Physical Chemistry)	75				4
	CHY 906	Research Project/ Industrial & field Training/ Survey	100	-	-	-	4
X	CHY 1001	Photochemistry/ Solid State	75				4
	CHY 1002	Environmental chemistry	75				4
	CHY 10031-10034	Paper Elective	75				4
	CHY 10041-10044	Paper Elective	75				4
	CHY 1005	Practical (Inorganic, Organic, & Physical Chemistry)	75				4
	CHY 1006	Project/Dissertation	100	-	-	-	4
		Grand Total	2500				100

Note: Duration of practical examination shall be 16 Hrs. (8 Hrs. / day) in each semester

\* Internal assessment 25% weightage of a course which includes 10 Marks mid-term assessment, 10 marks assignment/ presentation of given project and 5 marks of attendance/ activities.

*Mays*  
*convener*



**M.Sc. VII<sup>th</sup> Semester**  
(Course Content)

**CHY - 701: Application of Computer in Chemistry**

1. Introduction to computers and computing,
2. Computer programming in FORTRAN / Basic
3. Programming in Chemistry
4. Use of Computer Programmes.

**CHY - 702: Inorganic Chemistry**

1. Stereochemistry and Bonding in Main Group Compounds,
2. Metal - Ligand Equilibrium in Solution,
3. Metal-Ligands Bonding,
4. Metal  $\pi$ -Complexes,
5. Bonding in metal

**CHY - 703: Organic Chemistry**

1. Nature of bonding in organic molecules:
2. Stereochemistry
3. Reaction mechanism- Structure and reactivity
4. Pericyclic Reactions

**CHY - 704: Physical Chemistry**

1. Mathematical concept for physical chemistry.
2. Quantum Chemistry
  - A. Introduction to Exact quantum mechanical results
  - B. Approximate methods
  - C. Angular momentum
  - D. Electronic structure of atoms
  - E. Molecular orbital theory
3. Thermodynamics:
  - A. Classical thermodynamics
  - B. Statistical thermodynamics:
  - C. Non Equilibrium thermodynamics

**CHY - 705: Minor Subject-**

Select one minor elective course as minor subject from any other faculty (except own faculty) or interdisciplinary subject as suggested in ordinance 2022.

**CHY - 706: Practical**

1. Organic Chemistry
- ~~2. Inorganic Chemistry~~
2. Physical Chemistry

**CHY - 707: Project/ Dissertation**

Student shall take research project/survey/industrial training under the supervision of the faculty and submit their progress report at the end of semester.



1. **Introduction to computers and computing:** Basic structure and functioning of computers with a PC as an illustrative example, Memory, I/O devices, secondary storage, computer language, operating systems with DOS as an example, introduction to UNIX and WINDOWS, data processing, principles of programming, algorithms and flow-charts. 8
  
2. **Computer programming in FORTRAN / Basic:** Elements of the computer language, constants and variables, operations and symbols, expressions, arithmetic assignment statement, input and output. Format statement, termination statements, and branching statements such as IF or GO TO statement. Logical variables double precision variables, subscripted variables and Dimension, DO statement, FUNCTION and SUBROUTINE, COMMON and DATA statements. 12
  
3. **Programming in Chemistry:** Development of small computer codes involving simple formulae in chemistry, such as Vander Waals equation, pH titration, kinetics, radioactive decay, evaluation of lattice energy and ionic radii from experimental data, linear simultaneous equations to solve secular equations within the Huckel's theory, elementary structural features such as bond lengths, bond angles, dihedral etc of molecules extracted from a database such as Cambridge data base. 15
  
4. **Use of Computer Programmes:** The students will learn how to operate a PC and how to run standard programmes and packages, execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programmes, monte carlo and molecular dynamics, programmes with data preferably from physical chemistry laboratory, further, the students will operate one or two or the packages such as MATLAB, EASYPLOT, LOTUS, FOXPRO, FOXPRO and Word processing software such as WORDSTAR/MS-WORD. 25

#### Books Suggested

- i. Computers and Common Sense, R. Hunt and J. Shelley, Prentice Hall,
- ii. Computational Chemistry, A.C. Norris.
- iii. Microcomputer Quantum Mechanics, J.P. Kilingbeck, Adam Hilger.
- iv. Computer Programming in FORTRAN IV. V. Rajaraman, Prentice Hall.
- v. An Introduction to Digital Computer Design, V. Rajaraman and T. Radhakrishnan, Prentice Hall.



1. **Stereochemistry and Bonding in Main Group Compounds:** VSEPR, Walsh diagram (tri- and penta- atomic molecules),  $d_{\pi}$ - $P_{\pi}$  bonds, Bent rule and energetics of hybridization, Reactions of atomic inversion, free radical mechanism, nucleophilic displacement, perry-pseudo rotation of covalently bonded molecules. 12
2. **Metal - Ligand Equilibria in Solution:** Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry. 8
3. **Metal-Ligands Bonding:** Crystal field splitting in an octahedral and tetrahedral field, factors affecting the crystal field stabilizing energy, consequence of crystal field splitting, Dynamic & Static John-Teller Effect, Application and Limitation of crystal field theory, Site selection in spinals, molecular orbital theory, octahedral, tetrahedral and square planar complexes,  $\pi$ -bonding in octahedral complexes. 15
4. **Metal  $\pi$ -Complexes:** Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls, preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes, tertiary phosphine as ligands. 18
5. **Bonding in metal:** Introduction, Classical free electron theory, Molecular orbital approach, Valence bond approach, metallic conductivity, collision energy, metallic radii, distribution of metallic properties. 7

#### Books Suggested

- i. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
- ii. Inorganic Chemistry, J.E. Huhey, Harpes & Row,
- iii. Chemistry of the Elements, N.N. Greenwood and A. Earnshaw, Pergamon. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
- iv. Magnetochemistry, R.L. Carlin, Springer Verlag.
- v. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.

*Handwritten signatures and initials:*  
 [Signature: Mags]  
 [Signature: ...]  
 [Signature: ...]  
 [Signature: ...]



1. **Nature of bonding in organic molecules:** Delocalized chemical bonding-conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism, Aromaticity in benzenoid and non- benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of  $\pi$  -molecular orbitals, annulenes, anti-aromaticity, homo-aromaticity, PMO approach, bonds weaker than covalent – addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes. 10
  
2. **Stereochemistry:** Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity. Conformation of sugar, steric strain due to unavoidable crowding, elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis, asymmetric synthesis, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, stereochemistry of the compounds containing nitrogen, sulphur and phosphorus. 15
  
3. **Reaction mechanism- Structure and reactivity:** Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects, hard and soft acids and bases, generation, structure, stability and reactivity of carbocations, free radicals, carbenes, benzyne and nitrenes, effect of structure on reactivity-resonance and field effects, steric effect, quantitative treatment, the Hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation. 15
  
4. **Pericyclic Reactions:** Molecular orbital symmetry, Frontier orbitals of ethylene, 1, 3-butadiene, 1,3,5-Hexatriene and allyl system, classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams, FMO and PMO approach, Electrocyclic reactions-conrotatory and disrotatory motions,  $4n$  and  $4n + 2$  systems,  $2 + 2$  addition of ketenes, 1, 3dipolar cycloadditions and cheletropic reactions. Sigmatropic rearrangements- suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3-and 5,5-sigmatropic rearrangements, claisen, cope and aza- cope 20

*Handwritten signatures and initials:*  
 Maye  
 [Signature]  
 [Signature]  
 [Signature]  
 [Signature]



rearrangements, fluxional tautomerism, Ene reaction.

### Books Suggested

- i. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
- ii. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum.
- iii. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman. 3.
- iv. Structure and Mechanism in Organic Chemistry, C. K. Ingold, Cornell University Press.
- v. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall. 5.
- vi. Modern Organic Reactions, H. O. House, Benjamin.
- vii. Principles of Organic Synthesis, R. O. C. Noman and J. M. Coxon, Blackie Academic & Professional
- viii. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.
- ix. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan.
- x. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International,
- xi. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.



1. Mathematical Concept for Physical Chemistry

10

- A. Basic rules of differentiation, integration and logarithm
- B. Partial differentiation
- C. Exact and inexact differentiation with their applications in thermodynamic properties
- D. Addition and multiplication of Matrix
- E. Permutation and Combination.
- F. Probability

2. Quantum Chemistry

25

- A. **Introduction to exact quantum mechanical results:** The Schrodinger equation and the postulates of quantum mechanics, discussion of solutions of the Schrodinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.
- B. **Approximate methods:** The variation theorem, linear variation principle, perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the helium atom.
- C. **Angular momentum:** Ordinary angular momentum, generalized angular momentum, Eigen functions for angular momentum, Eigen values of angular momentum, operator using ladder operators, addition of angular momenta, spin, anti-symmetry and Pauli's exclusion principle.
- D. **Electronic structure of atoms:** Electronic configuration, Russell- Saunders terms and coupling schemes, Slater-Condon parameters, term separation energies of the  $p^n$  configuration, term separation energies for the  $d^n$  configurations, magnetic effects: spin-orbit coupling and Zeeman splitting, introduction to the methods of self-consistent field, the virial theorem.
- E. **Molecular orbital theory:** Huckel theory of conjugated systems, bond order and charge density calculations, applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc, introduction to external Huckel theory.



### 3. Thermodynamics:

- A. Classical thermodynamics:** Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies, partial molar free energy, partial molar volume and partial molar heat content and their significances, determinations of these quantities, concept of fugacity and determination of fugacity. Non-ideal systems: Excess functions for non-ideal solutions, activity, activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions, determinations of activity and activity coefficients, ionic strength, application of phase rule to three component systems, second order phase transitions.
- B. Statistical thermodynamics:** Concept of distribution, thermodynamic probability and most probable distribution, Ensemble averaging, postulates of ensemble averaging, canonical, grand canonical and micro canonical ensembles, corresponding distribution laws (Using Lagrange's method of undetermined multipliers), partition functions-translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions, applications of partition functions, heat capacity behaviour of solids- chemical equilibria and equilibrium constant in terms of partition functions, Fermi-dirac statistics, distribution law and applications to metal, bose- einstein statistics-distribution law and application to helium.
- C. Non Equilibrium thermodynamics:** Thermodynamic criteria for non- equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g. heat flow, chemical reaction etc), transformations of the generalized fluxes and forces, non-equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

#### Books Suggested

- i. Physical Chemistry, P.W. Atkins, ELBS.
- ii. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill,
- iii. Quantum Chemistry, Ira N. Levine, Prentice Hall.
- iv. Coulson's Valence, R. McWeeny, ELBS.
- v. Chemical Kinetics, K. J. Laidler, McGraw-Hill,
- vi. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose,



McMillan

- vii. Micelles, Theoretical and Applied Aspects, V. Morol, Plenum
  - viii. Modern Electrochemistry Vol. I and Vol. II, J.O.M. Bockris and A.K.N. Reddy, Plenum.
- Introduction to Polymer Science, V.R. Gowankar, N.V. Vishwanathan and J. Sridhar, Wiley  
Eastern

*Maya*  
*cyntia*  
*[Signature]*



### CHY - 705: Minor Elective Course

The candidates shall select any one subject from the following list as minor subject in first semester of post graduate course from any other faculty (except own faculty).

S.No.	Science	Arts	Commerce	Interdisciplinary
1.	Mathematical Biology	Tribal Culture and Heritage	Customer Relation Management	Ancient Medical Sciences
2.	Conservation and Water Resource	Principle of Administration and Implications	House Keeping and Hospitality	Traditional Medical Therapy
3.	Management Natural Resources and Conservation	Socio-Economics and Social Security	Share Market and Banking	Vedic Mathematics
4.	Pollution: Causes Archeological. Retail and Mitigation	Sites and Monuments	Retail Management and Accounting	Bio Medical Instrumentation and Health
5.	Computational Indian. Resources	Constitution	Insurance Policy and Finance	Disaster, Mitigation, & Management
6.	Organic and Natural Farming	Communication and Soft Skill		Mining Plan and Resource Mapping
7.	Computer Hardware Handling	Sanskrit Knowledge System		Water Treatment System
8.	Computer Software Handling	Translation and Trans creation		Climate Change Environmental Degradation
9.	Solar and Non Conventional Energy	Urban Economics and Planning		Medicinal and Aromatic Plants Cultivation, extraction and nutraceutical Values
10.	Cyber Crime	Actuarial Economics		
11.	Bee Keeping, Aquaculture and Fish Farming	Social Sector and Gender Economics		Non-Conventional Energy Resource
12.	Entrepreneurship in Microbial and Botanical Products	Environmental Economics		Soil and Water Testing



**1. Inorganic Chemistry**

**A. Lab Safety:**

- (i) Symbols of chemical bottles.
- (ii) Material Safety Data Sheet (MSDS).
- (iii) CAS (Chemical Abstract Service) number.
- (iv) Prevention of accident & first aid measurement.

**B. Qualitative and Quantitative Analysis:**

- (i) Less common metal ions - Ti, Mo, W, Ta, Zr, Th, V, U (two metal ions in cationic/anionic forms)
- (ii) Insolubles-oxides, sulphates and halides




**C. Chromatography:** Separation of cations and anions by-

- (i) Paper Chromatography
- (ii) Column Chromatography-Ion exchange.

**2. Organic Chemistry**

**A. Qualitative Analysis:**

Separation, purification and identification of compounds of binary mixture (one liquid and one solid) using TLC and column chromatography, chemical tests. IR spectra to be used for functional group identification.



### B. Quantitative Analysis:

- (i) Determination of the percentage or number of hydroxyl groups in an organic compound by acetylation method.
- (ii) Estimation of amines/phenols using bromated bromide solution/or acetylation method.

## 3. Physical Chemistry

### A. Chemical Kinetics:

- (i) Determination of the effect of (a) Change of temperature, (b) Change of concentration of reactants and catalyst, and (c) Ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reactions.
- (ii) Determination of the velocity constant of hydrolysis of an ester/ionic reaction in micellar media.
- (iii) Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine clock reaction.
- (iv) Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidised by per-sulphate ion).
- (v) Oscillatory reaction.





### Books Suggested

- i. Inorganic Experiments, J. Derek Woollins, VCH.
- ii. Microscale Inorganic Chemistry, Z. Szafran, R. M. Pike and M. M. Singh, Wiley.
- iii. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Van Nostrand.
- iv. Vogel's Textbook of Quantitative Analysis, revised. J. Bassett. R.C. Denney, G.H. Jeffery and J. Mendham, ELBS.
- v. Synthesis and Characterization of Inorganic Compounds. W.L. Jolly, Prentice Hall.
- vi. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall.
- vii. Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C. Heath.
- viii. Systematic Qualitative Organic Analysis. H. Middleton, Edward Arnold.
- ix. Handbook of Organic Analysis, Qualitative and Quantitative. H. Clark, Edward Arnold.
- x. Vogel's Textbook of Practical Organic Chemistry. A.R. Tatchell. John Wiley.
- xi. Practical Physical Chemistry, A.M. James and F. E. Prichard. Longman
- xii. Findley's Practical Physical Chemistry, B.P. Levitt. Longman.
- xiii. Experimental Physical Chemistry, R.C. Dasand, B. Behera, Tata Mc Graw Hill.



**Marks Distriution****Max. Marks**

1. Inorganic Experiment	20
2. Organic Experiment	20
3. Physical Experiment	20
4. Record	8
5. Viva- voce	7

**Total- 75**



**M.Sc. – VIII<sup>th</sup> Semester**

(Course Content)

**CHY - 801: Inorganic Chemistry, Group theory**

1. Reaction mechanism of transition metal complexes
2. Electronic spectra and magnetic properties of transition metal complexes
3. Metal-Clusters
4. Group theory

**CHY - 802: Organic Chemistry**

1. Aliphatic Nucleophilic substitution
2. Aliphatic Electrophilic substitution
3. Aromatic Electrophilic substitution
4. Aromatic Nucleophilic substitution
5. Free radical reactions
6. Addition to Carbon-Carbon multiple bonds
7. Addition to Carbon – Hetero multiple bonds
8. Elimination Reactions

**CHY - 803: Physical Chemistry**

1. Chemical Dynamics
2. Surface Chemistry
  - (a) Adsorption
  - (b) Micelle
  - (c) Macromolecules
3. Electrochemistry

**CHY - 804: Spectroscopy**

1. Microwave spectroscopy
2. Vibrational spectroscopy
  - A. Infrared spectroscopy
  - B. Raman spectroscopy
3. Electronic spectroscopy
  - A. Atomic spectroscopy
  - B. Molecular spectroscopy
4. Magnetic resonance spectroscopy
  - a. Nuclear Magnetic resonance spectroscopy
  - b. Nuclear Quadrupole resonance spectroscopy
5. X-ray Diffraction

**CHY - 805: Practical (Inorganic, Organic Chemistry & Physical Chemistry)**

**CHY - 806: Project/Dissertation**

Students continue his/her research project/survey/industrial training under the supervision of the faculty and submit the dissertation for evaluation at the end of semester.



1. **Reaction mechanism of transition metal complexes:** Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favor of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage, substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reaction, redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer-sphere type reactions, cross reactions and Marcus-hush theory, inner sphere type reactions. 20
  
2. **Electronic spectra and magnetic properties of transition metal complexes:** Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes ( $d^1$ - $d^9$  states), calculations of  $Dq$ ,  $B$  and  $\beta$  parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover. 18
  
3. **Metal-Clusters:** Higher boranes, carboranes, metalloboranes and metallocarboranes, metal carbonyl and halide clusters, compounds with metal-metal multiple bonds. 12
  
4. **Symmetry and group theory in chemistry:** symmetry elements and symmetry operation, definition of group, subgroup, relation between orders of a finite group and its subgroup, conjugacy relation and classes, point symmetry group, Schoenflies symbols, group multiplication table, representations of groups by matrices (representation for the  $C_n$ ,  $C_{nv}$ ,  $C_{nh}$ ,  $D_{nh}$  etc groups to be worked out explicitly). character tables and their use, spectroscopy. 10

#### Books Suggested

- i. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
- ii. Inorganic Chemistry, J.E. Huhey, Harpes & Row,
- iii. Chemistry of the Elements, N.N. Greenwood and A. Earnshaw, Pergamon. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
- iv. Magnetochemistry, R.L. Carlin, Springer Verlag.
- v. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.
- vi. Chemical Applications of Group Theory, F. A. Cotton, Wiley, India.

*Handwritten signatures and initials:*  
 May 1999  
 cymp  
 [Other illegible signatures]



1. **Aliphatic Nucleophilic substitution:** The  $S_N^2$ ,  $S_N^1$ , mixed  $S_N^2$  and  $S_N^1$ , and SET mechanism, the neighboring group mechanism, neighboring group participation by  $\sigma$  and  $\Pi$  bonds, anchimeric assistance, classical and non-classical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements, application of NMR spectroscopy in the detection of carbocations, the  $S_N^i$  mechanism, nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon, reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity. 12
  
2. **Aliphatic Electrophilic substitution:** Biomolecular mechanism- $SE^2$  and  $SE^1$ , The  $SE^i$  mechanism, electrophilic substitution accompanied by double bond shifts, effect of substrates, leaving group and solvent polarity on the reactivity. 5
  
3. **Aromatic Electrophilic substitution:** The arenium ion mechanism, orientation and reactivity, energy profile diagrams, the ortho/para ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrate and electrophiles, diazonium coupling, vilsmeier reaction, Gatterman Koch reaction. 6
  
4. **Aromatic Nucleophilic substitution:** The  $S_NAr$ ,  $S_N1$ , benzyne and  $S_{RN}1$  mechanisms, reactivity-effect of substrate structure, leaving group and attacking nucleophile, the Von Richter, Sommelet-Hauser and Smiles rearrangements. 5
  
5. **Free radical reactions:** Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighboring assistance, reactivity for aliphatic and aromatic substrates at a bridgehead, reactivity in the attacking radicals, the effect of solvents on reactivity. allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, free radical rearrangement, Hunsdiecker reaction. 8
  
6. **Addition to Carbon-Carbon multiple bonds:** Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and 7

*Handwritten signatures and initials:*  
 [Signature] [Initials] [Signature] [Signature] [Signature]



chemoselectivity, orientation and reactivity, addition to cyclopropane ring, hydrogenation of double and triple bonds, hydrogenation of aromatic rings, hydroboration, Michael reaction, Sharpless asymmetric epoxidation.

- 7. Addition to Carbon – Hetero multiple bonds:** Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles, addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, Wittig reaction, mechanism of condensation involving enolates-aldol, Knoevenagel, Claisen, Mannich, benzoin, Perkin and Stobbe Reactions. Hydrolysis of esters and amides, ammonolysis of esters. 12
- 8. Elimination Reactions:** The  $E^2$ ,  $E^1$  and  $E^1c_b$  mechanisms and their spectrum, orientation of the double bond, reactivity - effects of substrate structures, attacking base, the leaving group and the medium, mechanism and orientation in pyrolytic elimination. 5

#### Books Suggested

- i. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
- ii. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum.
- iii. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman. 3.
- iv. Structure and Mechanism in Organic Chemistry, C. K. Ingold, Cornell University Press.
- v. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall. 5.
- vi. Modern Organic Reactions, H. O. House, Benjamin.
- vii. Principles of Organic Synthesis, R. O. C. Noman and J. M. Coxon, Blackie Academic & Professional
- viii. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.
- ix. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan.
- x. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International,
- xi. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.



**1. Chemical dynamics:**

20

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory, ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions. Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chloride reactions) and oscillatory reactions (Belousov- Zhabotinsky reaction), homogeneous catalysis, kinetics of enzyme reaction, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method. Dynamics of molecular motions, probing the transition state, dynamics of barrierless chemical reactions in solution, dynamics of unimolecular reactions (Lindmann- Hinshelwood and Rice-Ramsperger- Kassel-Marcus [RRKM], theories of unimolecular reactions)

**2. Surface Chemistry:**

20

1. **Adsorption:** Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (electro-kinetic phenomenon), and catalytic activity surfaces.
2. **Micelles:** Surface active agents, classification of surface active agents, micellization, Hydrophobic interaction, Critical Micellar Concentration (CMC), Factors affecting the CMC of Surfactants, Counter Ion Binding to Micelles, Thermodynamics of Micellization-Phase Separation and Mass Action Models, Solubilization, Micro Emulsion, Reverse micelles.
3. **Macromolecules:** Polymer-Definition, Types of Polymers, Electrically conducting, Fire Resistant, Liquid Crystal Polymers, Kinetics of Polymerization, Mechanism of Polymerization, Molecular Mass, Number and Mass Average Molecular Mass, Molecular Mass Determination (Osmometry, viscometry, Diffusion and light scattering methods), Sedimentation, Chain Configuration of Macromolecules, Calculation of Average Dimensions of Various Chain Structures.

*Handwritten signatures and initials:*  
 [Signature] [Initials] [Signature] [Signature]



3. **Electrochemistry:** Electrochemistry of solutions, Debye-Huckel-Onsager electro treatment and its extension, ion solvent interactions, Debye-Huckel- Jerum mode, Thermodynamics of electrified interface equations, Derivation of electro-capillarity, Lippmann equations (surface excess), Methods of determination, structure of electrified interfaces, Guoy -Chapman, Stern, Graham- Devanathan-mottwatts, Tobin, Bockris, Devanathan models, over potentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot, quantum aspects of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling, semiconductor interfaces-theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces, effect of light at semiconductor solution interface.

4. **Electrocatalysis** – Influence of various parameters, hydrogen electrode. bioelectrochemistry, threshold membrane phenomena, Nernst-Plank equation, Hodges-polarography theory, Ilkovic equation, half wave potential and its significance, introduction to corrosion, homogenous theory, forms of corrosion, monitoring and prevention methods for corrosion

#### Books Suggested

- i. Physical Chemistry, P.W. Atkins, ELBS.
  - ii. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill,
  - iii. Quantum Chemistry, Ira N. Levine, Prentice Hall.
  - iv. Coulson's Valence, R. McWeeny, ELBS.
  - v. Chemical Kinetics, K. J. Laidler, McGraw-Hill,
  - vi. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan
  - vii. Micelles, Theoretical and Applied Aspects, V. Morol, Plenum
  - viii. Modern Electrochemistry Vol. I and Vol. II, J.O.M. Bockris and A.K.N. Reddy, Plenum.
- Introduction to Polymer Science, V.R. Gowankar, N.V. Vishwanathan and J. Sridhar, Wiley Eastem.

*cyant*  
*hays*  
*hays*



1. **Microwave Spectroscopy:** classification of molecules, molecular requirement for rotational spectra, the molecule as a rigid rotor, non-rigid rotor, effect of isotopic substitution on the transition frequencies, intensities, stark effect, nuclear and electron spin interaction and effect of external field, application. 4
2. **Vibrational Spectroscopy:** 12
  - A. **Infrared Spectroscopy:** linear harmonic oscillator, features of vibrational- rotational spectra, vibrational energies of diatomic molecules, zero point energy, frequency, force constant and bond strengths, molecules as an harmonic oscillator, morse potential energy diagram, the interaction of rotations and vibrations, molecules as vibrating rotator: fine structure of infra-red bands, P, Q and R branches, breakdown of oppenheimer approximation, vibration of polyatomic molecules, selection rules, normal modes of vibration, group frequencies, overtones, Thermal distribution of vibrational & rotational levels, factors affecting the band positions and intensities, analysis and application of infrared spectroscopy.
  - B. **Raman Spectroscopy:** Classical and Quantum theories of Raman effect, pure rotational, vibrational and vibrational-rotational Raman spectra, coherent anti stokes and stokes lines, selection rules, mutual exclusion principle, resonance Raman spectroscopy, infrared vs. Raman spectroscopy.
3. **Electronic Spectroscopy:** 12
  - A. **Atomic Spectroscopy:** structure of atoms, atomic quantum number, energies of atomic orbital, electronic angular momentum, vector representation of momenta and vector coupling, spectra of hydrogenatom and alkali metal atoms.
  - B. **Molecular Spectroscopy:** Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Frank Condon principle, electronic spectra of polyatomic molecules, predissociation, emission spectra, radioactive and non-radioactive decay, internal conversion, spectra of transition metal complexes, charge transfer spectra.
4. **Magnetic Resonance Spectroscopy:** 20
  - A. **Nuclear Magnetic Resonance Spectroscopy:** Nuclear spin, interaction between spin and a magnetic field, nuclear resonance, shielding of magnetic nuclei, chemical

*Handwritten signatures and scribbles at the bottom of the page.*



shift and its measurements, factors influencing chemical shift, de-shielding, spin-spin interactions, factors influencing coupling constant 'J', classification to AX, A<sub>2</sub>, AMX, ABC etc, spin decoupling, basic idea about instrument, NMR studies of nuclei other than proton-<sup>13</sup>C, <sup>19</sup>F and <sup>31</sup>P, FTNMR, advantages of FTNMR, use of NMR in medical diagnostics.

**B. Nuclear Quadrupole Resonance Spectroscopy:** Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting, applications.

**5. X-ray diffraction:** Bragg condition, miller indices, laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern, structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density, phase problem, description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramchandran diagram.

12

### Books Suggested

- i. Physical Methods for Chemistry, R.S. Drago, Saunders Company.
- ii. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS
- iii. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
- iv. Progress in Inorganic Chemistry vol., 8. ed., F.A. Cotton, vol., 15, ed. S.J. Lippard, Wiley.
- v. Transition Metal Chemistry ed. R.L. Carlin vol. 3, Dekker
- vi. Inorganic Electronic Spectroscopy.. A.P.B. Lever, Elsevier. 6.
- vii. NMR, NOR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
- viii. Practical NMR Spectroscopy, M.L Martin, J.J. Delpeuch and G.J. Martin, Heyden.
- ix. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Mornill, John Wiley
- x. Introduction to NMR Spectroscopy, R. J. Abraham, J. Fisher and P. Loftus, Wiley
- xi. Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall,
- xii. Spectroscopic Methods in Organic Chemistry, D. H. Williams, I. Fleming, Tata McGraw-Hill,



## 1. Inorganic Chemistry

### Qualitative and Quantitative Analysis:

- (i) Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. involving volumetric and gravimetric methods

## 2. Organic Chemistry

### Organic Synthesis:

- i. Acetylation: Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography
- ii. Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol
- iii. Grignard reaction: Synthesis of triphenylmethanol from benzoic acid
- iv. Aldol condensation: Dibenzal acetone from benzaldehyde
- v. Sandmeyer reaction: p-Chlorotoluene from p-toluidine
- vi. Acetoacetic ester Condensation: Synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation.
- vii. Cannizzaro reaction: 4-Chlorobenzaldehyde as substrate
- viii. Friedel Crafts Reaction:  $\beta$ -Benzoyl propionic acid from succinic anhydride and benzene
- ix. Aromatic electrophilic substitutions: Synthesis of p-nitroaniline and p-bromoaniline.

The Products may be characterized by Spectral Techniques



### 3. Physical Chemistry

#### A. Phase Equilibria:

- i. Determination of congruent composition and temperature of a binary system  
(e.g. diphenylamine-benzophenone system)
- ii. Determination of glass transition temperature of a given salt (e.g.,  $\text{CaCl}_2$ )  
conductometrically.
- iii. To construct the phase diagram for three component system (e.g. chloroform  
acetic acid-water).

#### B. Solutions:

- i. Determination of molecular weight of non-volatile and non-electrolyte/electrolyte  
by cryoscopic method and to determine the activity coefficient of an electrolyte.
- ii. Determination of the degree of dissociation of weak electrolyte and to study the  
deviation from ideal behavior that occurs with a strong electrolyte.





### Books Suggested

- i. Inorganic Experiments, J. Derek Woollins, VCH.
- ii. Microscale Inorganic Chemistry, Z. Szafran, R. M. Pike and M. M. Singh, Wiley.
- iii. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Van Nostrand.
- iv. Vogel's Textbook of Quantitative Analysis, revised. J. Bassett. R.C. Denney, G.H. Jeffery and J. Mendham, ELBS.
- v. Synthesis and Characterization of Inorganic Compounds. W.L. Jolly, Prentice Hall.
- vi. The Systematic Identification of Organic Compounds, R L. Shriner and D. Y Curtin.
- vii. Semimicro Qualitative Organic Analysis, N. D. Cheronis, J. B. Entrikin and E. M. Hodnett.
- viii. Experimental Organic Chemistry, M. P. Doyle and W. S. Mungall Small Scale Organic Preparations, P. J. Hill.
- ix. Practical Physical Chemistry, A.M. James and, F. E. Prichard. Longman.
- x. Findley's Practical Physical Chemistry, B.P. Levitt. Longman.
- xi. Experimental Physical Chemistry, R.C. Das and B. Behera, TataMc Graw Hill.



**Marks Distriution****Max. Marks**

i. Inorganic Experiment	20
ii. Organic Experiment	20
iii. Physical Experiment	20
iv. Record	8
v. Viva- voce	7

**Total- 75**



## M.Sc. IX<sup>th</sup> Semester

(Course Content)

### CHY - 901: Application of Spectroscopy

1. Inorganic Spectroscopy
  - A. Vibrational Spectroscopy
  - B. Electron Spin Resonance Spectroscopy
  - C. Nuclear Magnetic Resonance of Paramagnetic Substances in Solution
  - D. Mössbauer Spectroscopy
2. Organic Spectroscopy
  - A. Ultraviolet and Visible Spectroscopy
  - B. Infrared Spectroscopy
  - C. Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD)
  - D. Nuclear Magnetic Resonance Spectroscopy V Carbon-13 NMR Spectroscopy
  - E. Mass Spectrometry

### CHY - 902: Biochemistry

1. Bioinorganic Chemistry
  - A. Metal Ions in Biological Systems
  - B. Na/K<sup>+</sup> Pump
  - C. Bioenergetics and ATP Cycle
  - D. Transport and Storage of Dioxygen
  - E. Electron Transfer in Biology
2. Bioorganic Chemistry
  - A. Enzymes
  - B. Mechanism of Enzyme Action
  - C. Kinds of Reactions Catalysed by Enzymes
  - D. Co-Enzyme Chemistry
  - E. Enzyme Models
3. Biophysical Chemistry
  - A. Biological Cell and its Constituents
  - B. Bioenergetics
  - C. Thermodynamics of Biopolymer Solutions



**D. Diffraction Methods**

**CHY - 903: Elective Paper** (Select any one paper)

CHY 9031: Analytical techniques

CHY 9032: Liquid State

CHY 9033: Bioinorganic and Supramolecular Chemistry

CHY 9034: Organic Synthesis I

**CHY 904: Elective Paper** (Select any one paper)

CHY 9041: Analytical Chemistry

CHY 9042: Organotransition Metal Chemistry

CHY 9043: Natural Product

CHY 9044: Advance Quantum Chemistry

**CHY 905: Practical (Organic, Inorganic & Physical Chemistry)**

**CHY - 906: Project/ Dissertation**

Student shall take research project/survey/industrial training under the supervision of the faculty and submit the progress report at the end of semester.

*Handwritten signatures:*  
nagg  
R  
D  
my  
ST  
upth



1. Inorganic Chemistry

**A. Vibrational spectroscopy:** Symmetry and shapes of  $AB_2$ ,  $AB_3$ ,  $AB_4$ ,  $AB_5$  and  $AB_6$ , Mode of bonding of ambidentate ligands, ethylenediamine and diketonato complexes, Application of resonance Raman spectroscopy particularly for the study of active sites of metalloproteins.

**B. Electron Spin Resonance Spectroscopy:** Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to transition metal complexes (having one unpaired electron) including biological systems and to inorganic free radicals such as  $PH_4$ ,  $F^-$  and  $[BH^-]$ .

**C. Nuclear Magnetic resonance of Paramagnetic substances in solution:** The contact and pseudo contact shifts, factors affecting nuclear relaxation, some applications including biochemical systems, an overview of NMR of metal nuclides with emphasis on  $^{195}Pt$  and  $^{119}Sn$  NMR.

**D. Mossbauer Spectroscopy:** Basic principles, spectral parameters and spectrum display, application of the technique to the studies of (1) bonding and structures of  $Fe^{2+}$  and  $Fe^{3+}$  compounds including those of intermediate spin, (2)  $Sn^{+2}$  and  $Sn^{+4}$  compounds- nature of M-L bond, coordination number, structure and (3) detection of oxidation state and inequivalent MB atoms.

2. Organic Chemistry

**A. Ultraviolet and Visible Spectroscopy:** Various electronic transitions (185-800 nm), Beer-Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds, steric effects in biphenyls.



- B. Infrared Spectroscopy:** instrumentation and sample handling, 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, FTIR, IR of gaseous, solids and polymeric materials. 5
- C. Optical rotatory dispersion and Circular dichroism:** Definition, deduction of absolute configuration, octant rule for ketones. 3
- D. Nuclear Magnetic resonance spectroscopy:** General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling, stereochemistry, hindered rotation, Karplus curve-variation of coupling constant with dihedral angle, simplification of complex spectra-nuclear magnetic double resonance, contact shift reagents, solvents effects, Fourier transform technique, nuclear overhauser effect, resonance of other nuclei-F, P. 10
- E.  $^{13}\text{C}$  NMR Spectroscopy:** General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants, Two dimension NMR Spectroscopy – COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques 5
- F. Mass Spectroscopy:** 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. 8



### Books Suggested

- i. Physical Methods for Chemistry, R.S. Drago, Saunders Company.
- ii. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS
- iii. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
- iv. Progress in Inorganic Chemistry vol., 8. ed., F.A. Cotton, vol., 15, ed. S.J. Lippard, Wiley.
- v. Transition Metal Chemistry ed. R.L. Carlin vol. 3, Dekker
- vi. Inorganic Electronic Spectroscopy.. A.P.B. Lever, Elsevier. 6.
- vii. NMR, NOR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
- viii. Practical NMR Spectroscopy, M.L Martin, J.J. Delpuech and G.J. Martin, Heyden.
- ix. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Mornill, John Wiley
- x. Introduction to NMR Spectroscopy, R. J. Abraham, J. Fisher and P. Loftus, Wiley
- xi. Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall,
- xii. Spectroscopic Methods in Organic Chemistry, D. H. Williams, I. Fleming, Tata McGraw-Hill,

### CHY - 902: BIOCHEMISTRY

60 Hrs.

- |  |   |
|--|---|
| 1. Metal ions in biological systems: Essential and trace metals.   | 2 |
| 2. Na <sup>+</sup> /K <sup>+</sup> Pump: Role of metals ions in biological processes,  | 3 |
| 3. Bioenergetic and ATP Cycle: DNA polymerization, glucose storage, metal complexes in transmission of energy, chlorophylls, photosystem I and photosystem II in cleavage of water, model systems.       | 6 |
| 4. Transport and storage of Dioxygen: Heme protein and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper | 8 |
| 5. Electron Transfer in biology: Structure and function of metalloproteins in electron   | 6 |



transport processes-cytochromes and iron-sulphur proteins, synthetic models.

6. **Enzymes:** Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation, nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site – directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition. 6
7. **Mechanism of enzyme action:** transition state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion, examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, Lysozyme and carboxypeptidase A. 3
8. **Kinds of reactions catalysed by enzymes:** Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes, transfer of sulphate, addition and elimination reactions, enolic intermediates in isomerization reactions,  $\alpha$ -cleavage and condensation, some isomerization and rearrangement reactions, Enzyme catalysed carboxylation and decarboxylation. 6
9. **Co-Enzyme Chemistry:** Cofactors as derived from Vitamins, coenzymes, prosthetic groups, apoenzymes, structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate,  $\text{NAD}^+$ ,  $\text{NADP}^+$ , FMN, FAD, lipoic acid, vitamin B12, mechanism of reactions catalysed by the above cofactors. 4
10. **Enzyme models:** Host guest chemistry, chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality, biomimetic chemistry, crown ethers, cryptates, cyclodextrins, cyclodextrin-based enzyme models, calixarenes, ionophores, micelles, synthetic enzymes or synzymes. 4
11. **Biological cell and its constituents:** Biological cell, structure and functions of proteins, enzymes, DNA and RNA in living systems, Helix coil transition. 2
12. **Bioenergetics:** Standard free energy change in biochemical reactions, exergonic, endergonic, hydrolysis of ATP, synthesis of ATP from ADP. 3
13. **Thermodynamics of biopolymer solutions:** Thermodynamics of biopolymer 4



solutions, osmotic pressure, membrane equilibrium, muscular contraction and energy generation in mechanochemical system.

**14. Diffraction methods:** Light scattering, low angle X-ray scattering, X-ray diffraction and photo correlation spectroscopy, ORD

3

### Books Suggested

- i. Principles of Bioinorganic Chemistry. S.J. Lippard and J.M. Berg, University Science Books.
- ii. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
- iii. Inorganic Biochemistry vols I and II. ed. G.L. Eichhorn, Elsevier.
- iv. Progress in Inorganic Chemistry. Vols 18 and 38 ed. J.J. Lippard, Wiley.
- v. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer Verlag.
- vi. Understanding Enzymes, Trevor Palmer, Prentice Hall,
- vii. Enzyme Chemistry: Impact and Applications, Ed. Collin J Suckling, Chapman and Hall.



## CHY - 903: Elective Papers I

60 Hrs.

### CHY - 9031: Analytical Techniques

1. Significant figures; Determinate and Indeterminate errors, absolute and relative errors, error curves, minimization of errors; precision and accuracy, determination of accuracy; mean, median and mode; standard deviation. 8
2. Principles, instrumentation and applications of the following techniques: 15
  - i. Complexometric, Chelatometric and Non-aqueous titration.
  - ii. Potentiometric and Conductometric Titrations.
  - iii. Polarography and Amperometry
  - iv. Coulometry and Voltametry (With special reference to cyclic voltametry and Anodic Stripping voltametry).
3. Principles and applications of solvent extraction and ion exchangeresins. 12
4. Fundamental principles of chromatography. Principles, instrumentation and applications of column chromatography, paper chromatography, thin layer chromatography, gas chromatography, radial chromatography and HPLC. 15
5. Techniques and principles of Thermal Analysis: TGA, DTA and DSC. 10

### CHY - 9032: Liquid State

60 Hrs.

1. General Properties of Liquids: 13
  - a) Liquids as dense gases, liquids as disordered solids, some thermodynamic relations, internal pressure and its significance in liquids. Equations of state and critical constants. Different types of intermolecular forces in liquids, different potential functions for liquids, additivity of pair potential approximation.
  - b) A classical partition function for liquids, correspondence principle, configuration configuration properties.



- |   |    |
|---|----|
| 2. <b>Theory of Liquids:</b> Theory of liquids, partition function method or model approach; single cell models, communal energy and entropy, LTD model, significant structure model.   | 9  |
| 3. <b>Distribution Function and Related Equations:</b> Radial distribution function method, equation of state in terms of RDF. Molecular distribution functions, pair distribution function. Relationship between pair distribution function and pair potential function. The IBG equation, the HNC equation, the PY equation, cluster expansion. | 14 |
| 4. <b>Methods for Structure Determination and Computational Techniques:</b><br>Spectroscopic techniques for liquid dynamic, structure studies, Neutron and X-ray scattering spectroscopy.<br>Computation Techniques-Monte, Carlo and molecular dynamics methods.  | 12 |
| 5. <b>Supercooled and Ionic Liquids:</b> Supercooled and ionic liquids, theories of transport properties; non Arrhenius behaviour of transport properties, Cohen-Tumbull free volume model, configurational entropy model, Macedo-Litovitz hybrid model, glass transition in supercooled liquids.   | 12 |

### Books Suggested

- i. An Introduction to Liquid State, P.A. Egelstalf, Academic Press.
- ii. The Dynamic Liquid State, A.F.M. Barton, Longman
- iii. Introduction to Statistical Thermodynamics. T.L. Hill, Addison Wiley.
- iv. The Liquid State, J.A. Pryde.
- v. Significant Liquid Structures, H. Eyring and MS. John

### CHY - 9033: Bioinorganic Supramolecular Chemistry

60 Hrs.

- |  |    |
|--|----|
| 1. <b>Metal Storage Transport and Biomineralization:</b> Ferritin, transferrin, and siderophores   | 5  |
| 2. <b>Calcium in Biology:</b> Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins                     | 6  |
| 3. <b>Metalloenzymes:</b> Zinc enzymes - carboxypeptidase and carbonic anhydrase. Iron enzymes - catalase, peroxidase and cytochrome P-450. Copper enzymes - superoxide dismutase. | 20 |



Molybdenum oxatransferase enzymes - xanthine oxidase. Coenzyme vitamin B12

- |   |           |
|---|-----------|
| <b>4. Metal-Nucleic Acid Interactions:</b> Metal ions and metal complex interactions. Metal complexes - nucleic acids   | <b>6</b>  |
| <b>5. Metals in Medicine:</b> Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs         | <b>5</b>  |
| <b>6. Supramolecular Chemistry:</b>   | <b>12</b> |
| i. Concepts and language.   |           |
| ii. Molecular recognition: Molecular receptors for different types of molecules including arisonic substrates, design and synthesis of coreceptor molecules and multiple recognition. |           |
| iii. Supramolecular reactivity and catalysis.   |           |
| iv. Transport processes and carrier design.   |           |
| v. Supramolecular devices. Supramolecular photochemistry, supramolecular electronic, ionic and switching devices. Some example of self-assembly in supramolecular chemistry           |           |

#### Books Suggested

- i. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
- ii. Bio-norganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
- iii. Inorganic Biochemistry vols I and II. ed. G.L. Eichhom, Elsevier.
- iv. Progress Inorganic Chemistry. Vols 18 and 38 ed. J.J. Lippard, Wiley.
- v. Supramolecular Chemistry. J.M. Lehn, VCH.

#### CHY - 9034: Organic Synthesis – I

- |  |           |
|--|-----------|
| <b>A. Organometallic Reagents:</b> Principle, preparations, properties and applications of the following inorganic synthesis with mechanistic details- | <b>30</b> |
| i. Group I and II metal organic compounds  |           |
| ii. Li, Mg, Hg, Cd, Zn and Ce compounds.   |           |



- iii. Transition metals
- iv. Cu, Pd, Ni, Fe, Co, Rh, Cr and Ti compounds.
- v. Other elements
- vi. S, Si, B and I compounds.

#### B. Oxidation:

10

Introduction. Different oxidative processes. Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated and unactivated). Alcohols, diols, aldehydes, ketones, ketals and carboxylic acids, Amines, hydrazines, and sulphides. Oxidations with ruthenium tetroxide, iodobenzene diacetate and thallium nitrate.

#### C. Reduction:

10

Introduction. Different reductive processes.

Hydrocarbons- alkanes, alkenes, alkynes and aromatic rings.

Carbonyl compounds-aldehydes, ketones, acids and their derivatives. Exposides. Nitro, nitroso, azo and oxime groups.

Hydrogenolysis.

#### D. Rearrangements:

10

General mechanistic considerations-nature of migration, migratory aptitude, memory effects.

A detailed study of the following rearrangements.

Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofman, Curtius, Schmidt, Baeyer-Viliger, Shapiro reaction.

#### Books Suggested

- i. Modern Synthetic Reactions, H.O. House, W. A. Benjamin.
- ii. Some Modern Methods of Organic Synthesis, W. Camuthers, Cambridge Univ. Press.
- iii. Advanced Organic Chemistry, Reactions Mechanisms and Structure, J. March,



John Wiley. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, Blackie Academic & Professional.

- iv. Advanced Organic Chemistry Part B. F. A. Carey and R. J. Sundberg, Plenum Press.
- v. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.

### CHY - 904: ELECTIVE PAPER- II

#### CHY - 9041: Analytical Chemistry

60 Hrs.

1. **Introduction:** Role of analytical chemistry. Classification of analytical methods-classical and instrumental. Types of instrumental analysis. Selecting an analytical method. Neatness and cleanliness. Laboratory operations and practices. Analytical balance. Techniques of weighing, errors. Volumetric glassware-cleaning and calibration of glassware. Sample preparations dissolution and decompositions. Gravimetric techniques. Selecting and handling of reagents. Laboratory notebooks. Safety in the analytical laboratory. 12
2. **Errors and Evaluation:** Definition of terms in mean and median. Precision-standard deviation, relative standard deviation. Accuracy-absolute error, relative error. Types of error in experimental data determinate (systematic), indeterminate (or random) and gross. Sources of errors and the effects upon the analytical results. Methods for reporting analytical data. Statistical evaluation of data-indeterminate errors. The uses of statistics 7
3. **Food Analysis:** Moisture, ash, crude protein, fat, crude fibre, carbohydrates, calcium, potassium, sodium and phosphate. Food adulteration-common adulterants in food, contamination of food stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food products. Extraction and purification of sample. HPLC. Gas chromatography for organophosphates. Thin-layer chromatography for identification of chlorinated pesticides in food products. 12
4. **Analysis of Water Pollution:** Origin of waste water, types, water pollutants and their 12



effects. Sources of water pollution domestic, industrial, agricultural soil and radioactive wastes as sources of pollution. Objectives of analysis-parameter for analysis-colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen. Heavy metal pollution-public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. General survey of instrumental technique for the analysis of heavy metals in aqueous systems. Measurements of DO, BOD and COD. Pesticides as water pollutants and analysis. Water pollution laws and standards.

#### 5. Analysis of Soil, Fuel, Body Fluids and Drugs:

- i. Analysis of soil: moisture, pH, total nitrogen, phosphorus, silica, lime, magnesia, manganese, sulphur and alkali salts.
- ii. Fuel analysis: solid, liquid and gas. Ultimate and proximate analysis-heating values grading of coal. Liquid fuels-flash point, aniline point, aclane number and carbon residue. Gaseous fuels-producer gas and water gas-calorific value.
- iii. Clinical chemistry: Composition of blood collection and preservation of samples. Clinical analysis. Serum electrolytes, blood glucose, blood urea nitrogen, uric acid, albumin, globulins, barbiturates, acid and alkaline phosphatases. Immunoassay: principles of radio immunoassay (RIA) and applications. The blood gas analysis trace elements in the body.
- iv. Drug analysis: Narcotics and dangerous drugs. Classification of drugs. Screening gas and thin-layer chromatography and spectrophotometric measurements.

#### Books Suggested

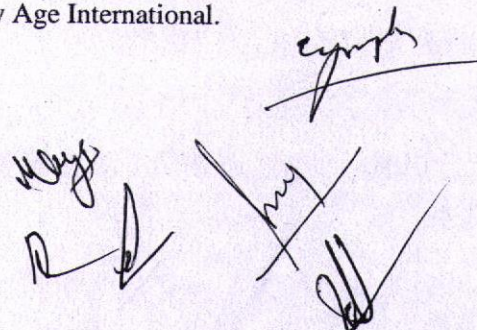
- i. Analytical Chemistry, G.D. Christian, J. Wiley.
- ii. Fundamentals of Analytical Chemistry, D.A. Skoog, D M. West and F.J. Holler, W. B. Saunders.
- iii. Analytical Chemistry-Principles, J.H. Kennedy, W. B. Saunders
- iv. Analytical Chemistry-Principles and Techniques. L.G. Harps, Prentice Hall.
- v. Principles of Instrumental Analysis, DA Skoog and J.L. Loary, W. B. Saunders.
- vi. Principles of instrumental Analysis, D.A. Skoog, W. B. Saunders
- vii. Quantitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
- viii. Environmental Solution Analysis, S.M. Khopkar, Wiley Eastern
- ix. Basic Concepts of Analytical Chemistry, S M. Khopkar, Wiley Eastern
- x. Handbook of instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.



1. **Alkyls and Aryls of Transition Metals:** Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis 5
2. **Compounds of Transition Metal-Carbon Multiple Bonds:** Alkylidenes, alkylidynes, low valent carbenes and carbynes- synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions or the ligands, role in organic synthesis. 12
3. **Transition Metal  $\pi$ -Complexes:** Transition metal  $\pi$ -complexes with unsaturated organic molecules, alkenes, alkynes, ailyl, diene, dienyl, arene and trienyl complexes, preparations, properties, nature of bonding and structural features. Important reactions relating to nucleophilic and electrophilic attack on ligands and to organic synthesis 18
4. **Transition Metal Compounds with Bonds to Hydrogen:** Transition metal compounds with bonds to hydrogen. 3
5. **Homogeneous Catalysis:** Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of clefins (oxo reaction), oxopalladation reactions, activation of C-H bond. 14
6. **Fluxional Organometallic Compounds:** Fluxionality and dynamic equilibria in compounds such as n olefin,  $n^3$  allyl and dieny! complexes 8

**Books Suggested**

- i. Principles and Application of Organotransition Metal Chemistry, J.P. Colanan, LS. Heysdus. J.R. Norton and H.G. Finke, University Science Books:
- ii. The Organometallic Chemistry of the Transition Metals, R.H. Crabtree, John Wiley
- iii. Motalo-organic Chemistry, A.J. Pearson. Wiley.
- iv. Organometallic Chemistry, R.C. Mehrotra and A. Singh, New Age International.





1. **Terpenoids and Carotenoids:** Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Citral, Geraniol,  $\alpha$ -Terpeneol, Menthol, Farnesol, Zingiberene, Santonin, Phytol, Abiatic acid and  $\beta$ -Carotene. 15
2. **Alkaloids:** 15  
Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following:  
Ephedrine, (+)- Coniine, Nicotine, Atropine, Quinine and Morphine.
3. **Steroids:** 15  
Occurrence, nomenclature, basic skeleton, Diels-Alder reaction and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Bile acids, Androsterone, Testosterone, Estrone, Progesterone, Aldosterone. Biosynthesis of steroids.
4. **Plant Pigments:** 7  
Occurrence, nomenclature and general methods of structure determination, isolation and synthesis of Apigenin, Luteoline, Quercetin, Myricetin, Quercetin-3-glucoside, Vitexin, Diadzein, Butein, Aureusin, Cyanidin-7-arabinoside, cyanidin, Hirsutidin. Biosynthesis of flavonoids : Acetate pathway and Shikimic acid pathway.
5. **Porphyrins:** Structure and synthesis of Hemoglobin and Chlorophyll 3
6. **Prostaglandins:** Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE<sub>2</sub> and PGF<sub>2</sub> 3
7. **Pyrethroids and Rotenones:** 3  
Synthesis and reactions of Pyrethroids and Rotenones. (For structure elucidation, emphasis is to be placed on the use of spectral parameters wherever possible).

*Handwritten signatures and initials:*  
 - A signature that appears to be "Cyril".  
 - Several other initials and signatures, including one that looks like "Magg".



**CHY – 9044: Advanced Quantum Chemistry****60 Hrs.**

(Pre-requisite: Mathematics at least up to First Year B.Sc. level is necessary. At least one PU among 4 students should be available)

- |    |  |    |
|----|--|----|
| 1. | <b>Theoretical and Computational Treatment of Atoms and Molecules, Hartree-Fock Theory:</b> Review of the principles of quantum mechanics Born-Oppenheimer approximation Slater-Condon rules. Hartree-Fock equation Koopmans and Brinkman theories, Roothaan equation, Gaussian basis sets.      | 12 |
| 2. | <b>Configuration Interaction and MC-SCF:</b> Introduction to CI, full and truncated CI theories, size consistency. Introductory treatment of coupled cluster and MC-SCF methods.   | 12 |
| 3. | <b>Semi-Empirical Theories:</b> A review of the Huckel, EHT and PPP treatments, ZDO approximation, detailed treatment of CNDO and INDO theories. A discussion of electronic energies and properties. An introduction to MCPAC and AMI with hands on experience on personal computers             | 12 |
| 4. | <b>Density Functional Theory:</b> Derivation of Hohenberg-Kohn theorem Kohn-Sham formulation, N. and V representables; review of the performance of the existing (eg. Slater Xa and other methods) and non-local functionals, treatment of chemical concepts with the density functional theory. | 12 |
| 5. | <b>Computer Experiments:</b> Computer experiments using quantum chemistry software packages such as GAUSSIAN GAMESS/MOPAC and modeling software eg MM2/AMBER/CHARM.  | 12 |

**Books Suggested**

- i. Modern Quantum Chemistry. N.S. Oetung and A. Sabo, McGraw Hill.
- ii. Methods of Molecular Quantum Mechanics, R. Mc Weeny and B.T. Sutcliffe Academic Press.
- iii. Density Functional Theory of Atoms and Molecules. R.G. Parr and W. Yang, Oxford
- iv. Exploring Chemistry with Electron Structure Methods, J.B. Foresman and E. Frisch, Gaussian Inc.
- v. Semi-empirical MO Theory, Pople and D.L. Beveridge.

Handwritten signatures and initials, including 'Maya', 'cyngta', and other illegible marks.



**1. Inorganic Preparations:**

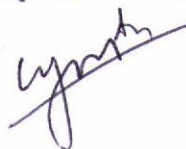
Preparation of selected inorganic compounds and their studies by I.R., Electronic spectra, Mossbauer, E.S.A. and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds-

- i.  $\text{VO}(\text{acac})_2$
- ii.  $\text{TiO}(\text{C}_9\text{H}_8\text{NO})_2 \cdot 2\text{H}_2\text{O}$
- iii.  $\text{cis-K}[\text{Cr}(\text{C}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$
- iv.  $\text{Na}[\text{Cr}(\text{NH}_3)_2(\text{SCN})_4]$
- v.  $\text{Mn}(\text{acac})_3$
- vi.  $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]$
- vii. PrussianBlue, Turnbull'sBlue.
- viii.  $\text{Co}(\text{NH}_3)_6][\text{Co}(\text{NO}_2)_6]$ .
- ix.  $\text{cis-}[\text{Co}(\text{trien})(\text{NO}_2)_2]\text{Cl} \cdot \text{H}_2\text{O}$
- x.  $\text{Hg}[\text{Co}(\text{SCN})_4]$
- xi.  $[\text{Co}(\text{Py})_2\text{Cl}_2]$
- xii.  $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$
- xiii.  $\text{Ni}(\text{DMG})_2$
- xiv.  $[\text{Cu}(\text{NH}_3)_4]\text{SO}_4 \cdot \text{H}_2\text{O}$

**2. Organic Chemistry**

**A. Organic Qualitative Analysis:**

Separation, purification and identification of the components of a mixture of three organic





compounds (three solids or two liquids and one solid, two solids and one liquid), using tic for checking the purity of the separated compounds, chemical analysis, IR, PMR and mass spectral data.

## **B. Extraction of Organic Compounds from Natural Sources**

- i. Isolation of caffeine from tea leaves.
- ii. Isolation of casein from milk (the students are required to try some typical color reactions of proteins).
- iii. Isolation of lactose from milk (purity of sugar should be checked by TLC and PC and Rf value reported).
- iv. Isolation of nicotine dipicrate from tobacco. Isolation of cinchonine from cinchona bark
- v. Isolation of piperine from black pepper.
- vi. Isolation of lycopene from tomatoes.
- vii. Isolation of  $\beta$ -carotene from carrots.
- viii. Isolation of oleic acid from olive oil (involving the preparation of complex with urea and separation of linoleic acid).
- ix. Isolation of eugenol from cloves.
- x. Isolation of (+) limonine from citrus rinds

## **C. Paper Chromatography:**

Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of Rf values.





### 3. Physical Chemistry:

#### A. Error Analysis and Statistical Data Analysis:

Errors, types of errors, minimization of errors, error distribution curves, precision, accuracy and combination; statistical treatment for error analysis, student 't' test, null hypothesis, rejection criteria, F. & Q test; linear regression analysis, curve fitting.  
Apparatus: burette, pipette and standard flask.

#### B. Adsorption:

- i. To study surface tension-concentration relationship for solutions (Gibb's equation).
- ii. Study the adsorption of acidic acid on charcoal and draw the Freundlich isotherm

#### Book Suggested

- i. Inorganic Experiments, J. Derek Woollins, VCH.
- ii. Microscale Inorganic Chemistry, Z. Szafran, R. M. Pike and M. M. Singh, Wiley.
- iii. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Van Nostrand.
- iv. Vogel's Textbook of Quantitative Analysis, revised. J. Bassett. R.C. Denney, G.H. Jeffery and J. Mendham, ELBS.
- v. Synthesis and Characterization of Inorganic Compounds. W.L. Jolly, Prentice Hall.
- vi. The Systematic Identification of Organic Compounds, R L. Shriner and D. Y Curtin.
- vii. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall.
- viii. Macro scale and Micro scale Organic Experiments, K.L. Williams on, D.C. Heath.
- ix. Systematic Qualitative Organic Analysis. H. Middleton, Edward Arnold.



- x. Handbook of Organic Analysis, Qualitative and Quantitative. H. Clark, Adward Arnold.
- xi. Vogel's Textbook of Practical Organic Chemistry. A.R. Tatchell .John Wiley.
- xii. Practical Physical Chemistry, A.M. James and F, E. Prichard. Longman.
- xiii. Findley's Practical Physical Chemistry, B.P. Levitt. Longman.
- xiv. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata Mc Graw Hill.
- xv. Organametallic Synthesis, J J. Fisch and R B. King, Academic.
- xvi. Experimental Physical Chemistry, D. P. Shoemaker, C. W. Garland and J. W. Niber, McGraw Hill Interscience.
- xvii. Experiments in Physical Chemistry, J. C, Ghosh, Bharati Bhavan.

#### Marks Distriution

#### Max. Marks

1. Inorganic Experiment	20
2. Organic Experiment	20
3. Physical Experiment	20
4. Record	8
5. Viva- voce	7

**Total- 75**



## M.Sc. - X<sup>th</sup> Semester

(Course Content)

### CHY - 1001: Photochemistry/ Solid State

#### 1. Photochemistry

- Photochemical Reactions. Determination of Reaction Mechanism
- Photochemistry of Alkenes
- Photochemistry of Carbonyl Compounds
- Photochemistry of Aromatic Compounds Miscellaneous Photochemical Reactions

#### 2. Solid State Chemistry

- Solid State Reactions Crystal Defects and Non-Stoichiometry
- Electronic Properties and Band Theory
- Organic Solids

### CHY - 1002: Environmental Chemistry

- Environment
- Hydrosphere
- Soils
- Atmosphere
- Industrial Pollution
- Environmental Toxicology

### CHY - 1003: Elective Paper (Select any one paper)

CHY 10031: Medicinal Chemistry

CHY 10032: Chemistry of Materials

CHY 10033: Organic Synthesis II

CHY 10034: Physical Organic Chemistry

### CHY - 1004: Elective Paper (Select any one paper)

CHY 10041: Polymer Chemistry

CHY 10042: Computation Chemistry

CHY 10043: Photoinorganic Chemistry

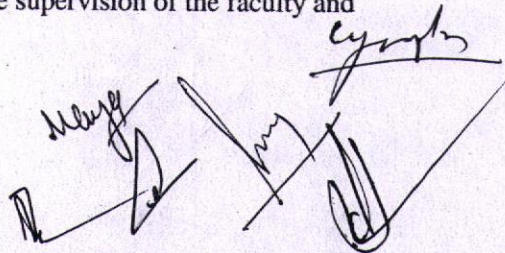
CHY 10044: Heterocyclic Chemistry

### CHY - 1005: Practical (~~Inorganic, Organic & Physical Chemistry~~)

*Instrumental method  
of analysis & organic synth.*

### CHY - 1005: Project/ Dissertation

Student shall take research project/survey/industrial training under the supervision of the faculty and submit the progress report at the end of semester.





## CHY - 1001: Photochemistry and Solid State Chemistry

60 Hrs.

### 1. Photochemistry:

30 Hrs.

- A. Photochemical Reactions:** Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry. 4
- B. Determination of reaction mechanism:** Classification, rate constants and life times of reactive energy states-determination of rate constants of reactions, effect of light intensity on the rate of photochemical reactions, types of photochemical reactions-photo dissociation, gas-phase photolysis. 4
- C. Photochemistry of alkenes:** Intramolecular reactions of the olefinic bond-geometrical isomerization, cyclic reactions, rearrangement of 1,4- and 1,5-dienes. 6
- D. Photochemistry of carbonyl compounds:** intramolecular reactions of the carbonyl compounds- saturated, cyclic and acyclic,  $\beta$ - $\gamma$  Unsaturated and  $\alpha$ - $\beta$  unsaturated compounds, cyclohexadienones, intermolecular cycloaddition reactions-dimerisation and oxetane formation. 8
- E. Photochemistry of aromatic compounds:** isomerization, addition and substitutions. 4
- F. Miscellaneous photochemical reactions:** Photo-fries reactions of anilides, photo-fries rearrangement, Barton reaction, singlet molecular oxygen reactions, photochemical formation of smog, photo degradation of polymers, photochemistry of vision. 4

### 2. Solid State Chemistry:

30 Hrs.

- A. Solid State reactions:** General principles, experimental procedures, co-precipitation as a precursor to solid-state reactions, kinetics of solid-state reactions. 4
- B. Crystal Defects and Non-Stoichiometry:** Perfect and imperfect crystals, 6



intrinsic and extrinsic defects-point defects, line and plane defects,

Vacancies- Schottky defects and Frenkel defects, thermodynamics of Schottky and Frenkel defect formation, color centers, non-Stoichiometry and defects.

**C. Electronic properties and band theory:** Metals, insulators and semiconductors, electronic structure of solid-band theory, band structure of metals, insulators and semiconductor, intrinsic and extrinsic semiconductors, doping semiconductor, p-n-junction, super conductors, optical properties-optical properties - optical reflectance, photoconduction-photoelectric effects, magnetic properties-classification of materials: quantum theory of paramagnetic-cooperative phenomena-magnetic domains, hysteresis.

**D. Organic solids:** Electrically conducting solids, organic charge transfers complex, organic metals, new superconductors.

#### Book Suggested

- i. Fundamentals of Photochemistry, K. K. Rohtagi-Mukherji. Wiley. Eastern Essentials of Molecular Photochemistry, A. Gilbert and J. Baggott, Blackwell Scientific Publication
- ii. Molecular Photochemistry, N. J. Turro, W. A. Benjamin.
- iii. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill
- iv. Photochemistry, R. P. Kundall and A. Gilbert, Thomson Nelson.
- v. Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.
- vi. Solid State Chemistry and its Applications, A.R. West, Plenum.
- vii. Principles of the Solid State, H.V. Keer, Wiley Eastern.
- viii. Solid State Chemistry, N.B. Hannay,
- ix. Solid State Chemistry, D.K. Chakrabarty, New Age International,

*Handwritten signatures and initials:*  
A large signature at the top right, possibly "cyndi".  
Below it, several other signatures and initials, including one that looks like "may" and another that looks like "A".



## CHY - 1002: Environmental Chemistry

60 Hrs.

1. **Environment:** Introduction, composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere, and biogeochemical cycles of C, N, P, S and O, Bio distribution of elements. 8
2. **Hydrosphere:** Chemical composition of water bodies – lakes, streams, rivers and wetlands etc Hydrological cycle. Aquatic pollution-inorganic, organic, pesticides, agricultural, industrial and sewage, detergents, oil spills and oil pollutants, water quality parameters-dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms, water quality standards, Analytical methods for measuring BOD, DO, COD, F, OILS, METALS (As, Cd, Cr, Hg, Pb, Se), Residual chloride and chlorine demand, purification and treatment of water. 12
3. **Soils:** Composition, micro and macronutrients, pollution-fertilizers, pesticides, plastics and metals, waste treatment. 6
4. **Atmosphere:** Chemical Composition of Atmosphere-particles, ions and radical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons, greenhouse effect, acid rain, air pollution controls and their chemistry, analytical methods for measuring air pollutants, continuous monitoring instruments. 8
5. **Industrial pollution:** Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy, polymers, drugs etc, radionuclide analysis, disposal of wastes and their management. 12
6. **Environmental Toxicology:** Chemical solutions to environmental problems, bio-degradability, principles of decomposition, better industrial processes. 14

### Books Suggested

- i. Environmental Chemistry, S. E. Manahan, Lewis Publishers.
- ii. Environmental Chemistry, Sharma & Kaur, Krishna Publishers.



- iii. Environmental Chemistry, A. K. De, Wiley Eastern.
- iv. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern
- v. Standard Method of Chemical Analysis, F.J. Welcher Vol. III, Van Nostrand Reinhold Co
- vi. Environmental Toxicology. Ed. J. Rose, Gordon and Breach Science Publication.
- vii. Elemental Analysis of Airborne Particles. Ed. S. Landsberger and M. Creatchman, Gordon and Breach Science Publication.
- viii. Environmental Chemistry, C. Baird, W. H. Freeman.

### CHY-1003: Paper Elective I

60 Hrs.

#### CHY-10031: Medicinal Chemistry

15

##### 1. Drug Design:

Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR). factors affecting bioactivity, resonance, Inductive effect, isosterism, bio-leosteriem, spatial considerations. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptor interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials. Free-Wilson analysis, Hansch analysis, relationships between Free-Wilson and Hansch analysis. LD<sub>50</sub>, ED<sub>50</sub> (Mathematical derivations of equations excluded).

##### 2. Pharmacokinetics:

5

Introduction to drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention of uses of pharmacokinetics in drug development process.

##### 3. Pharmacodynamics:

5

Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation,

*Handwritten signatures and initials:*  
 [Signature] [Signature] [Signature] [Signature]



significance of drug metabolism in medicinal chemistry.

**4. Antineoplastic Agents:**

5

Introduction, cancer chemotherapy, special problems, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antibiotics and mitotic inhibitors. Synthesis of mechlorethamine, cyclophosphamido, melphalan, uracil, mustards, and 6 mercaptopurine. Recent development in cancer chemotherapy. Hormone and natural products.

**5. Cardiovascular Drugs:**

5

Introduction, cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators Synthesis of amyl nitrate, sorbitrate, diltiazem, quinidine, verapamil, methyldopa, atenolol oxyphenolol.

**6. Local Antiinfective Drugs:**

10

Introduction and general mode of action. Synthesis of sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, norfloxacin, dapsone, amino salicylic acid, isoniazid, ethionamide, ethambutal, fluconazole, econazole, griseofulvin, chloroquin and primaquin.

**7. Psychoactive Drugs- The Chemotherapy of Mind:**

7

Introduction, neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazepines, buspirone, neurochemistry of mental diseases. Antipsychotic drugs - the neuroleptics, antidepressants, butyrophenones, serendipity and drug development, stereochemical aspects of psychotropic drugs. Synthesis of diazepam, oxazepam, chlorazepam, alprazolam, phenytoin, ethosuximide, trimethadione, barbiturates, thiopental sodium, glutethimide

**8. Antibiotics:**

8

Cell wall biosynthesis, inhibitors, B-lactam rings, antibiotics inhibiting protein synthesis Synthesis of penicillin G, penicillin V. ampicillin, amoxycillin, chloramphenicol, cephalosporin, tetracyclin and streptomycin.

**Books Suggested**

- i. Introduction to Medicinal Chemistry, A Gringuage. Wiew-VCH.



- ii. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry. Ed Robert F.Dorge.
- iii. An Introduction to Drug Design, S. S. Pandeya and J. R. Dimmock, New Age International.
- iv. Burger's Medicinal Chemistry and Drug Discovery, Vol-1 (Chapter-9 and Ch-14). Ed. M. E. Wolff, John Wiley.
- v. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill.
- vi. The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.

## CHY-10032: Chemistry of Materials

60 Hrs.

### 1. Multiphase Materials:

5

Ferrous alloys; Fe-C phase transformations in ferrous alloys; stainless steels, non-ferrous alloys, properties of ferrous and non-ferrous alloys and their applications.

### 2. Glasses, Ceramics, Composites and Nanomaterials:

5

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

### 3. Thin Films and Langmuir-Blodgett Films:

5

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

### 4. Liquid Crystals:

10

Mesomorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases: smectic nematic transition and clearing temperature- homeotropic, planar and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic A and smectic C phases, optical properties of liquid

*Handwritten signatures and initials:*  
 Days  
 [Signature]  
 [Signature]  
 [Signature]



crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

**5. Polymeric Materials:**

5

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

**6. Ionic Conductors:**

8

Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel). vacancy mechanism, diffusion superionic conductors: phase transitions and mechanism of conduction in superionic conductors, examples and applications of ionic conductors.

**7. High T<sub>c</sub> Materials:**

10

Defect perovskites, high T<sub>c</sub> superconductivity in cuprates, preparation and characterization of 1-2-3 and 2-1-4 materials, normal state properties; anisotropy; temperature dependence of electrical resistance; optical phonon modes, superconducting state; heat capacity. coherence length, elastic constants, position lifetimes, microwave absorption-pairing and multi gap structures in high T<sub>c</sub> materials, applications of high T<sub>c</sub> materials.

**8. Materials for Solid State Devices:**

3

Rectifiers, transistors, capacitors -IV-V compounds, low-dimensional quantum structures: optical properties.

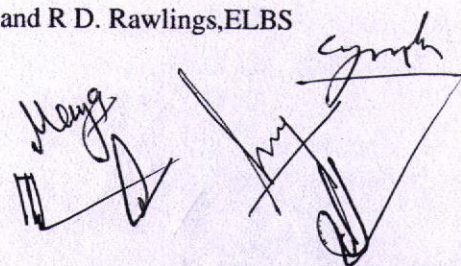
**9. Organic Solids, Fullerenes, Molecular Devices:**

9

Conducting organics, organic superconductors, magnetism in organic materials. Fullerenes-doped, fullerenes as superconductors. Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory and switches-sensors. Nonlinear optical materials: nonlinear optical effects. second and third order molecular hyperpolarisability and second order electric susceptibility- materials for second and third harmonic generation.

**Books Suggested**

- i. Solid State Physics, N.W. Ashcroft and ND, Marmin, Saunders College.
- ii. Material Science and Engineering, An Introduction, W.D. Calister, Wiley.
- iii. A Principles of the Solid State, H.V. Keer, Wiley Eastem.
- iv. Materials Science, J.C. Anderson, K.D. Leaver, JM. Alexander and R D. Rawlings, ELBS





- v. Thermotropic Liquid Crystals, Ed. G.W. Gray, John Wiley.
- vi. Handbook of Liquid Crystals, Keteer and Hatz, Chemie Verlag.

## CHN-10033: Organic Synthesis II

60 Hrs.

### 1) Disconnection Approach:

30

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

### 2) Protecting Groups:

12

Principle of protection of alcohol, amine, carbonyl and carboxyl groups.

### 3) One Group C-C Disconnections

3

Alcohols and carbonyl compounds, regioselectivity. Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.

### 4) Two Group C-C Disconnections

3

Diels-Alder reaction, 1,3-difunctionalised compounds, unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds, Michael addition and Robinson annulations.

### 5) Ring Synthesis

4

Saturated heterocycles, synthesis of 3-, 4-, 5- and 6-membered rings, aromatic heterocycles in organic synthesis.

### 6) Synthesis of Some Complex Molecules

8

Application of the above in the synthesis of following compounds: Camphor, Longifoline, Cortisone, Reserpine, Vitamin D, Juvabione, Aphidicolin and Fredericamycin A.

## BOOKS SUGGESTED

- i. Designing Organic Synthesis. S. Warren, Wiley.
- ii. Organic Synthesis- Concept, Methods and Starting Materials, J.Fuhrhop and G.



- Penzillien, Verlage VCH.
- iii. Some Modern Methods of Organic Synthesis. W. Carruthers, Cambridge Univ. Press',
  - iv. Modern Synthetic Reactions, H.O.House, W. A. Benjamin,
  - v. Advanced Organic Chemistry: Reactions, Mechanisms and Structure. J. March.Wiley ..
  - vi. Principles of Organic Synthesis. A. Norman and J. M. Coxon, Blackie Academic & Professional.
  - vii. Advanced Organic Chemistry Part B, F. A. Carey and A. J. Sundberg, Plenum Press

#### CHY-10034: Physical Organic Chemistry

60 Hrs.

#### 1. Concepts In Molecular Orbital (MO) and Valence Bond (VB) Theory:

10

Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Advanced techniques in PMO and FMO theory. Molecular mechanics, semi empirical methods and ab initio and density functional methods. Scope and limitations of several computational programmes.

Quantitative MO theory - Huckel molecular orbital (HMO) method as applied to ethene, allyl and butadiene. Qualitative MO theory Ionisation potential. Electron affinities. MO energy levels. Orbital symmetry. Orbital Interaction diagrams. MO of simple organic systems such as ethene, allyl, butadiene, methane and methyl group. Conjugation and hyperconjugation. Aromaticity.

Valence bond (VB) configuration mixing diagrams. Relationship between VB configuration mixing and resonance theory. Reaction profiles. Potential energy diagrams. Curve crossing model-nature of activation barrier in chemical reactions

#### 2. Principles of Reactivity:

5

Mechanistic significance of entropy, enthalpy and Gibb's free energy. Arrhenius equation. Transition state theory. Uses of activation parameters, Hammond's postulate, Bell-Evans Polanyi principle. Potential energy surface model. Marcus theory of electron transfer. Reactivity and selectivity principles.

#### 3. Kinetic Isotope Effect:

4

Handwritten signatures and initials, including 'cyndi' and 'Mou', are present at the bottom right of the page.



6

## 6

6

## 6

6

## 6

56

Handwritten notes: Henry Cynthia

6

Structural and electronic effects on S1 and S2 reactivity. Solvent effects Kinetic isotope effects. Intramolecular assistance. Electron transfer nature of S2 reaction. Nucleophilicity and S2 reactivity based on curve- crossing model. Relationship between polar and electron transfer reactions. Saw mechanism, Electrophilic reactivity, general mechanism, Kinetic S2-Ar reaction. Structural effects on rates and selectivity Curve-crossing approach to



electrophilic reactivity.

#### 9. Radical and Pericyclic Reactivity:

Radical stability, polar influences, solvent and steric effects. A curve crossing approach to radical addition, factors effecting barrier heights in additions, regioselectivity in radical reactions, Reactivity, specificity and periselectivity in pericyclic reactions.

#### 10. Supramolecular Chemistry:

Properties of covalent bonds bond length inter-bond angles, force constant, bond and molecular dipole moments Molecular and bond polarizability, bond dissociation enthalpy. entropy. Intermolecular forces, hydrophobic effects Electrostatic, induction, dispersion and resonance energy magnetic interactions. magnitude of interaction energy, forces between macroscopic bodies, medium effects Hydrogen bond Principles of molecular association and organization as exemplified in biological macromolecules ke enzymes nucleic acids, membranes and model systems like micelles and vesicles Molecular receptors and design principles Cryptands, cyclophanes. calixeranes, cyclodextrines. Supramolecular reactivity and catalysis. Molecular channels and transport processes. Molecular devices and nanotechnology.

#### Books Suggested

- i. Molecular Mechanics, U. Burkert and N. L. Allinger, ACS Monograph 177, 1982.
- ii. Organic Chemists' Book of Orbitals. L. Salem and W. L. Jorgensen, Academic Press.
- iii. Mechanism and Theory in Organic Chemistry, T. H. Lowry and K. C. Richardson, and Row
- iv. Introduction to Theoretical Organic Chemistry and Molecular Modeling, W. B. Smith, VCH, Weinheim.
- v. Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman.
- vi. Supramolecular Chemistry: Concepts and Perspectives, J. M. Lehn, VCH.
- vii. The Physical Basis of Organic Chemistry, H. Maskill, Oxford University Press.



## CHY-1004: Elective Papers II

### CHY-10041: Polymer Chemistry

60 Hrs.

#### 1. Basics:

8

Importance of polymers. Basic concepts: Monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers Polymerization: condensation, addition, radical chain-ionic and co-ordination and co polymerization. Polymerization conditions and polymer reactions. Polymerization In homogeneous and heterogeneous systems.

#### 2. Polymer Characterization:

14

Polydispersion-average molecular weight concept. Number, weight and viscosity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End-group, viscosity, light scattering, osmotic and ultracentrifugation methods. Analysis and testing of polymers chemical analysis of polymers, spectroscopic methods, X-ray diffraction study. Microscopy. Thermal analysis and physical testing-tensile strength. Fatigue, impact. Tear resistance, Hardness and abrasion resistance.

#### 3. Structure and Properties:

14

Morphology and order in crystalline polymers-configurations of polymer chains. Crystal structures of polymers. Morphology of crystalline polymers, strain-induced morphology. Crystallization and melting. Polymer structure and physical properties-crystalline melting point  $T_m$ -melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature,  $T_g$ -Relationship between  $T_m$  and  $T_g$ . effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

#### 4. Polymer Processing:

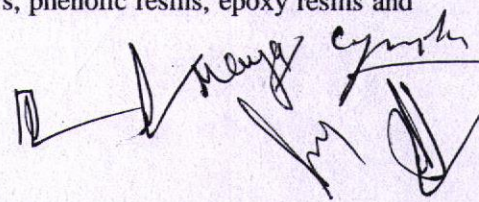
12

Plastics, elastomers and fibres. Compounding Processing techniques: Calendering, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming. reinforcing and fibre spinning.

#### 5. Properties of Commercial Polymers:

12

Polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and





silicone polymers. Functional polymers Fire retarding polymers and electrically conducting polymers. Biomedical polymers contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

### Books Suggested

1. Textbook of Polymer Science, F.W. Billmeyer Jr, Wiley.
2. Polymer Science, V.R. Gowariker, N.V. Viswanathan and J. Sreedhar, Wiley-Eastern.
3. Functional Monomers and Polymers, K. Takemoto, Y. Inaki and RM. Ottanbrite.
4. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
5. Physics and Chemistry of Polymers, J.M.G. Cowie, Blackie Academic and Professional.

### CHY - 10042: Computation Chemistry

60 Hrs.

#### 1. Fortran/C Programming and Numerical Methods:

15

Advanced programming features of FORTRAN/C. Basic theory, discussion of algorithms and errors for the following numerical methods. Examples from chemistry should be selected for illustrating the methods. The teacher may select ANY THREE of the following subtopics considering the background of students, available time etc.

##### A. Solution of Equations

Bisection, regular falsi, Newton-Raphson and related methods for solving polynomial and transcendental equations. Convergence. Errors and ill-conditioning.

##### B. Linear Simultaneous Equations

Gaussian elimination, Gauss-Seidel method, Gauss-Jordan method. Pivoting strategy. Errors and ill conditioning.

##### C. Eigenvalues and Matrix Diagonalization

Jacobi and Householder methods, analysis or errors.

##### D. Interpolation

Newton forward and backward difference, central differenced formulae. Lagrange and Hermite interpolation. Polynomial wiggle problem.

##### E. Numerical Differentiation

Solution of simple differential equations by Taylor series and Runge-Kutta methods

##### F. Numerical Integration

Newton-Cotes formulae, Romberg integration, errors in integration formulae. The students should develop computer programs for some of the above numerical methods



## 2. Running of Advanced Scientific Packages:

15

The students are expected to get hands on experience of running a few selected advanced level scientific software packages after & boot Introduction to the basic theory and methodology. ab initio quantum chemical packages such as GAUSSIAN GAMES with carefully designed exercises for illustrating various features of the packages Semi-empirical/Dynamics/Simulation packages such as MOPAC, CHARM, AMBER, QUANTA etc. Basic ideas on structure activity relation, drug and catalysis design etc.

## 3. Introduction to Networking and Search using Internet

10

## 4. Project:

20

The students will develop utilities such as analysis of spectra, simulation programmes which will supplement laboratory or theory exercises in physical, organic, inorganic chemistry or biochemistry. This list is only indicative and a variety of small projects designed by the teacher based on the interest of the student and capabilities should be worked out.

### Books Suggested

- i. Computational Chemistry, A.C. Norris, John Wiley.
- ii. Computer Programming in FORTRAN 77. R. Rajaraman, Prentice Hall.
- iii. Numerical Analysis, C. E. Frogberg, Macmilan.
- iv. Numerical Analysis A Practical Approach, M.J. Maron, John Wiley.
- v. Numerical Methods for Scientists and Engineers, H. M. Anta, Tata McGraw Hill.

## CHY-10043: Photoinorganic Chemistry

60 Hrs.

### 1. Basics of Photochemistry

30

Absorption, excitation, photochemical laws, quantum yield, electronically excited states life times-measurements of the times. Flash photolysis, stopped flow techniques. Energy dissipation by radiative and non-radiative processes, absorption spectra, Franck-Condon principle, photochemical stages-primary and secondary processes

### 2. Properties of Excited States

5

Structure, dipole moment, acid-base strengths, reactivity. Photochemical kinetics



calculation of rates of radiative processes. Bimolecular deactivation- quenching

### 3. Excited States of Metal Complexes

5

Excited states of metal complexes: comparison with organic compounds, electronically excited states of metal complexes, charge-transfer spectra, charge transfer excitations, methods for obtaining charge-transfer spectra

### 4. Ligand Field Photochemistry

5

Photosubstitution, photooxidation and photoreduction, ability and selectivity. Zero vibrational levels of ground state and excited state, energy content of excited state, zero zero spectroscopic energy, development of the equations for redox potentials of the excited states.

### 5. Redox Reactions by Excited Metal Complexes

10

Energy transfer under conditions of weak interaction and strong interaction-excimer formation conditions of the excited states to be useful as redox reactants, excited electron transfer metal complexes as attractive candidates (2,2-bipyridine and 1,10 phenanthroline complexes). Illustration of reducing and oxidising character of Ruthenium (pyridine) complex, comparison with Ferripyridyls: role of spin-orbit coupling-life time of these complexes. Application of redox processes of electronically excited states for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light

### 6. Metal Complex Sensitizers

5

Metal complex sensitizer, electron relay, metal colloid systems, semiconductor supported metal or oxide systems, water photolysis, nitrogen fixation and carbon dioxide reduction

### Books Suggested

- i. Concepts of Inorganic Photochemistry, A.W. Adamson and P.D. Fischauer, Wiley
- ii. Inorganic Photochemistry, J. Chem. Educ, vol 00, no. 10, 1003
- iii. Progress in Inorganic Chemistry, vol. 30, ed. J. Lipman Wiley.
- iv. Coordination Chem, Revs 1981, vol 39, 121, 131, 1975 15 321, 1000, 97, 313 5.
- v. Chemistry of Coordination Compounds, V. Batra and V. Caras, Academic Press 6.
- vi. Elements of inorganic Photochemistry G. J. Feraud Wiley



**1. Nomenclature of Heterocycles**

4

Replacement and systematic nomenclature (Hantzsch - Widman system) for monocyclic, fused and bridged heterocycles.

**2. Aromatic Heterocycles**

5

General chemical behavior of aromatic heterocycles, classification (structural type), criteria of aromaticity (bond lengths, ring current and chemical shifts in  $^1\text{H}$  NMR-spectra, empirical resonance energy, delocalization energy and Dewar resonance energy, diamagnetic susceptibility exaltations). Heteroaromatic reactivity and tautomerism in aromatic heterocycles

**3. Non Aromatic Heterocycles**

6

Strain -bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles with reference to molecular geometry, barrier to ring inversion, pyramidal inversion and 1,3-diaxial interaction. Stereo-electronic effects - anomeric and related effects. Attractive interactions - hydrogen bonding and intermolecular nucleophilic- electrophilic interactions.

**4. Heterocyclic Synthesis**

4

Principles of heterocyclic synthesis involving cyclization reactions and cycloaddition reactions.

**5. Small Ring Heterocycles**

5

Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, thiiranes, azetidines, oxetanes and thietanes

**6. Benzo Fused Five Membered Heterocycles**

5

Synthesis and reactions including medicinal applications of benzopyrroles, benzofurans and benzothiophenes

**7. Mesoionic Heterocycles**

5


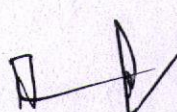
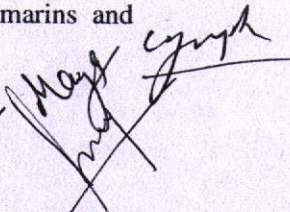
General classification, chemistry of some important meso-ionicheterocycles of type-A and B and their applications.

**8. Six Membered Heterocycles with One Heteroatom**

6

Synthesis and reactions of pyrylium salts and pyrones and their comparison with pyridinium & thiopyrylium salts and pyridones.

Synthesis and reactions of quinolininium and benzopyrylium salts, coumarins and

*Handwritten signatures and initials:*  
  
  




chromones

**9. Six-Membered Heterocycles with Two or More Heteroatoms**

5

Synthesis and reactions of diazines, triazines, tetrazines and thiazines

**10. Seven and Large Membered Heterocycles**

5

Synthesis and reactions of azepines, oxepines, thiepinines, diazepines, thiazepines, azocines, diazocines, dioxocines and dithiocines.

10

**11. Heterocyclic System Containing P, As, Sb and B**

**a) Heterocyclic rings containing phosphorus:**

Introduction; nomenclature, synthesis and characteristics of 5- and 6- membered ring systems- phosphorinanes, phosphorines, phospholanes and phospholes.

**b) Heterocyclic rings containing As and Sb:**

Introduction, synthesis and characteristics of 5 and 6- membered ring systems.

**c) Heterocyclic rings containing B:**

Introduction, Synthesis, reactivity and spectral characteristics of 3-, 5- and 6- membered ring systems.

**BOOKS SUGGESTED:**

- i. Heterocyclic Chemistry, Vol 1-3, A. A. Gupta. M. Kumar and V. Gupta, Springer Verlag
- ii. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme
- iii. Heterocyclic Chemistry, J. A. Joule, K. Mills and G.F. Smith, Chapman and Hall
- iv. Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific Technical
- v. Contemporary Heterocyclic Chemistry, G. A. Newkome and W. W. Paudler, Wiley-Inter Science
- vi. An Introduction to the Heterocyclic Compounds, A. M. Acheson, John Wiley
- vii. Comprehensive Heterocyclic Chemistry, A. A. Katritzky and C. W. Rees. eds. Pergamon Press



**1. Analysis of soil, water, & oil by using various parameters.**

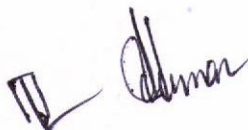
**2. Tools in Chemical Science:**

- A. Basic knowledge of some chemical tools to draw: Chemical structure, X-ray Crystallography & molecular modeling.
- B. Identification of material by instruments like UV, IR, NMR, XRD, SEM, TEM, BET & MASS-spectra.
- C. Chemical analysis by using pH meter, colorimeter, conductivity meter, polaro-meter & spectrophotometer.
- D. Estimation of metal in solution by colorimetry and spectrophotometry.

**3. Organic Chemistry**

**A. Multi-step Synthesis of Organic Compounds**

The exercises should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques-





(i) Photochemical reaction

Benzophenone  $\rightarrow$  Benzpinacol-Benzpinacolone

(ii) Beckmann rearrangement: Benzanilide from benzene

Benzene Benzophenone Benzophenone oxime  $\rightarrow$  Benzanilide

(iii) Benzilic acid rearrangement: Benzilic acid from benzoin

Benzoin Benzil  $\rightarrow$  Benzilic acid

(iv) Synthesis of heterocyclic compounds

Skraup synthesis: Preparation of quinoline from aniline

(v) Fisher -Indole synthesis:

Preparation of 2-phenylindole from phenyl-hydrazine.

(vi) Enzymatic synthesis

Enzymatic reduction: Reduction of ethyl acetoacetate using Bakers' yeast to yield

(vii) Enantiomeric excess of S (+) ethyl-3-hydroxybutanoate and determine its

optical purity. Biosynthesis of ethanol from sucrose

(viii) Synthesis using microwaves.

Alkylation of diethyl malonate with benzyl chloride,

(ix) Synthesis using phase transfer catalyst

Alkylation of diethyl malonate or ethyl acetoacetate with an alkyl halide.



### Books Suggested

- i. Inorganic Experiments, J. Derek Woollins, VCH.
- ii. Microscale Inorganic Chemistry, Z. Szafran, R. M. Pike and M. M. Singh, Wiley.
- iii. Practical Inorganic Chemistry, G. Marr and B. W. Rockett, Van Nostrand
- iv. The Systematic Identification of Organic Compounds, R L. Shriner and D. Y Curtin
- v. Semimicro Qualitative Organic Analysis, N. D. Cheronis, J. B. Entrikin and E. M. Hodnett
- vi. Experimental Organic Chemistry, M. P. Doyle and W. S. Mungall Small Scale Organic Preparations, P. J. Hill.
- vii. Practical Physical Chemistry, A.M. James and F. E. Prichard. Longman.
- viii. Findley's Practical Physical Chemistry, B.P. Levitt. Longman.
- ix. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.
- x. Organometallic Synthesis, J J. Fisch and R B. King, Academic.
- xi. Experimental Physical Chemistry, D. P. Shoemaker, C. W. Garland and J. W. Niber, McGraw Hill Inter science.
- xii. Experiments in Physical Chemistry, J. C. Ghosh, Bharati Bhavan.





### Marks Distriution

### Max. Marks

1. At least three practical from each unit  
carry 20 marks each.

60

2. Record

8

3. Viva- voce

7

**Total- 75**

*[Signature]*

*[Signature]*

*[Signature]*