Bundelkhand University, Jhansi

Board of Studies

In accordance with NEP-2020

(12)

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. Ajul Ansari	Memb.							
3-	Dr. Anilku	Membi.							
4.	Mayavesm	Memb.							
5-	Dr Ekta Pand	Expm Subj.							
6-	Dr Chitrag Gupta	Coordi nato.							

Comments

Internal members 1 2 Convenor 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 Anilkumar
Deptt of Chemistry
B.B.C. Jhansi

Dr Maya Verma
HOD
Deptt of Chemistry
Govt. Girls PG College Banda

(Dr. M.A. Ansari)

Ekta Pandey
(वाहय विषय विशेषज्ञ)

Dr. Chitra Gupta
(Co-ordinator)
Deptt. of Chemistry
Bundelkhand University

Convenor
5/07/22

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

SEMESTER	PAPER CODE	PAPER	THEORY (MARKS-75 MAX.)	INTENRAL (MARKS -25)			CREDIT
			75	25*			
			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)~~ Instru...	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.

Convenor

M.Sc. VIIth 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 π-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.

CHY - 701: Application of Computer in Chemistry — 60Hrs

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, arithemetic assignment statement, input and output. Format statement, termination statements, and branching statements such as IFor GO TO statement. Logical variables double precision variables, subscribed 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, numeriacal 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.

CHY - 702: Inorganic Chemistry

60Hrs

1. **Stereochemistry and Bonding in Main Group Compounds:** VSEPR, Walsh diagram (tri- and penta- atomic molecules), d_π -P_π 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, π -bonding in octahedral complexes. **15**

4. **Metal π-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 anddioxygen 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. Earnshow, 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.

CHY - 703: Organic Chemistry 60 Hrs.

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 π -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, asymmetricsynthesis, 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, benzynes and nitrenes, effect of structure on reactivity-resonance and field effects, steric effect, quantitative treatment, the Hammett equation and linear free energy relationship, substitutent 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 cheleotropic 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

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.

CHY - 704: Physical Chemistry — 60 Hrs.

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 ofsolutions 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-Condom 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, cyclopropeneyl radical, cyclobutadiene etc, introduction to external Huckel theory.

25

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 partion 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 statics-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. Levino, 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

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 Manageme nt	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 Finence	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 Econo mics		
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

CHY 706: Practical (Organic, Inorganic, & Physical Chemistry) **270 Hrs.**
(18 hrs /week)

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 - Tl, Mo, W, Ti, Zr, Th, V, U (two metal ions in cationic/anionicforms)

(ii) Insolubles-oxides, sulphates and halides

C. Chromatography: Separation of cations and anions by-

(i) Paper Chromatography

(ii) Column Chromatography-lon exchange.

2. Organic Chemistry

A. Qualitative Analysis:

Separation, purification and identification of compounds of binary mixture (oneliquid 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, Adward Arnold.

ix. Handbook of Organic Analysis, Qualitative and Quantitative. H. Clark, Adward 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. – VIIIth 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.

CHY - 801: Inorganic Chemistry and Group Theory — 60 Hrs.

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 β 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 ofa finite group and its subgroup, conjugacy relation and classes, point symmetry group, schonfiles 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 explicity). 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. Earnshow, 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, Willey, India.

CHY - 802: Organic Chemistry

60 Hrs.

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 σ and Π bonds, anchimeric assistance, classical and non-classical carbocations, phenonium ions, norbornyl system, commoncarbocation rearrangements, application of NMR spectroscopy in the detection of carbocations, the Sn^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, vilsmeir 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, Sommlet-Houser 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, Hunsdicker 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**

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 condensationr involving enolates-aldol, knovenagel, 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^1cb mechanisms and their spectrum, orientation of the double bond, reactivity - effects of substrate structures, attacking base, the leaving group and the medium, mechanismand 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.

CHY - 803: Physical Chemistry 60 Hrs.

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.

3. **Electrochemistry:** Electrochemistry of solutions, Debye-Huckel-Onsager electro treatment and its extension, ion solvent intractions, 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 solutioninterfaces, structure of double layer interfaces, effect of light at semiconductor solution interface. **15**

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 **5**

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. Levino, 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.

CHY - 804: Spectroscopy

60 Hrs.

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

shift and its measurements, factors influencing chemical shift, de-shielding, spin-spin interactions, factors influencing coupling constant 'J', classification to AX, A_2, AMX, ABC etc, spin decoupling, basic idea about instrument, NMR studies of nuclei other than proton-^{13}C, ^{19}F and ^{31}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, 1. Fleming, Tata McGraw-Hill,

CHN - 805: Practical (Inorganic, Organic, & Physical Chemistry) **270 Hrs.** (18 hrs/week)

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 columnchromatography

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: ß-Benzoyl propionic acid from succinic anhydride and benzene

ix. Aromatic electrophilic sustitutions: 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.,$CaCl_2$) 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. IXth 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 lons in Biological Systems
   - **B.** Na/K* 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 1

CHY 904: Elective Paper (Select any one paper)

CHY 9041: Analytical Chemistry

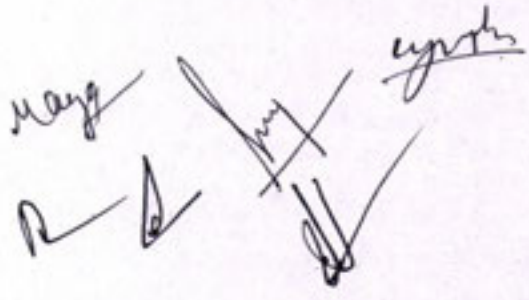
CHY 9042: Organotransition Metal Chemistry

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.



CHY - 901: Application of spectroscopy

60 Hrs.

1. Inorganic Chemistry **5**

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, $F^{\cdot}$ and $[BH]^{\cdot}$. **8**

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. **7**

D. Mossbauer Spectroscopy: Basic principles, spectral parameters and spectrum display, application of the technique to the studies of (1) bonding and structures of Fe2+ and Fe3+ 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. **6**

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. **3**

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 overhouser effect, resonance of other nuclei-F, P. **10**

E. **^{13}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 spectralfragmentation 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. 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, 1. Fleming, Tata McGraw-Hill,

CHY - 902: BIOCHEMISTRY

60 Hrs.

1. **Metal ions in biological systems:** Essential and trace metals. **2**

2. **Na+/k+ 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 ion-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:** transport state theory, orientation and steric effect, acid-dase 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, □-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, NAD^+, $NADP^+$, 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; standarddeviation. **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 Annodic 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. **Theory of Liquids:** Theory of liquids, partition function method or model approach; single cell models, communal energy and entropy, LTD model, significant structure model. **9**

3. **Distribution Function and Related Equations:** 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. **Methods for Structure Determination and Computational Techniques:** **12**

   Spectroscopic techniques for liquid dynamic, structure studies, Neutron and X-ray scattering spectroscopy.

   Computation Techniques-Monte, Carlo and molecular dynamics methods.

5. **Supercooled and Ionic Liquids:** 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. **Metal Storage Transport and Biomineralization:** Ferritin, transferrin, and siderophores **5**

2. **Calcium in Biology:** Calcium in living cells, transport and regulation, molecular aspects of intramolecular processes, extracellular binding proteins **6**

3. **Metalloenzymes:** 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

4. **Metal-Nucleic Acid Interactions:** Metal ions and metal complex interactions. Metal complexes - nucleic acids **6**

5. **Metals in Medicine:** Metal deficiency and disease, toxic effects of metals, metals used for diagnosis and chemotherapy with particular reference to anticancer drugs **5**

6. **Supramolecular Chemistry:** **12**

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

A. **Organometallic Reagents:** Principle, preparations, properties and applications of the following inorganic synthesis with mechanistic details- **30**

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 carboxyalic acids, Amines, hydrazines, and sulphides. Oxidations with ruthenium tetraoxide, 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. Modem 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.

CHY - 9042: Orgaotransition Metal Chemistry **60 Hrs.**

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 π –Complexes:** Transition metal π-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^{23} 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.

CHY – 9043: Natural products **60 Hrs.**

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, α-Terpeneol, Menthol, Farnesol, Zingiberene, Santonin, Phytol, Abiatic acid and β-Carotene. **15**

2. **Alkaloids:**

   Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradatin, classification based on nitrogen heterocyclic ring, role of alkeloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following: **15**

   Ephedrine, (+)- Conviine, Nicotine, Atropine, Quinine and Morphine.

3. **Steroids:** **15**

   Occurrence, nomenclature. basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Bile acids, Androsterone., Testosterone, Estrone, Progestrone, Aldosterone. Biosynthesis of steroids.

4. **Plant Pigments:** **7**

   Occurrence, nomenclature and general methods of structuredetermination, isolation and synthesis of Apigenin, Luteoline, Quercetin, Myrectin, Quercetin-3-glucoside, Vitexin, Diadzein, Butein, Aureusin I Cyandin-7-arabinoside, cyanidin, Hirsutidin. Biosynthesis of flavonoids : Acetate pathway and Shikimic acid pathway.

5. **Porphyrins:** Structure and synthesis of Hemoglobin and Chlorophyl **3**

6. **Prostaglandins:** Occurrence, nomenclature, classification, biogenesis and physiological effects. Synthesis of PGE_2 and PGF 2' **3**

7. **Pyrethroids and Rotenones:**

   Syathesis and reactions of Pyrethroids and Retenones. (For structtJre elucidation, emphasis is to be place on the use of spectral parameters wherever possible).

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

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

1. **Theoretical and Computational Treatment of Atoms and Molecules, Hartree-Fock Theory:** Review of the principles of quantum mechanics Bom-Oppenheimer approximation Sister-Condin rules. Hartree-Fock acuation Koopmans and Brifouin theories, Roothan equation, Gaussian basis sets. **12**
2. **Configuration Interaction and MC-SCF:** Introduction to Ci, full and truncated Cl theories, size consistency. Introductory treatment of coupled cluster and MC-SCF methods. **12**
3. **Semi-Empirical Theories:** 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. **Density Functional Theory:** Derivation of Hohenberg-Kohn thaorom Kohn-Sham formulation, N. and V representablises; review of the performance of the existiincal (eg. Sater Xa and other methods) and non-local functionals, treatment of chemical concepts with the density functional theory. **12**
5. **Computer Experiments:** Computer experiments using quantum chemistry software packages much as GAUSSIAN GAMESS/MOPAC and modeling software eg MM2/AMBER/CHARM. **12**

Books Suggested

i. Maden Quartien Chemistry. NS. Oetune and A. Sabo, McGow Hill.

ii. Methods of Molecular Quantum Mechanics, R. Mc Weeny and BT. Sutcliffe Academic Press.

iii. Density Functional Theory of Atoms and Molecules. R.G. Parr and W, Yang, Oxford

iv. Exploring g Chemistry with Electron Structure Mithos, JB Foresman and E frish, Goussian Inc.

v. Semi-empirical MO Theory, Pople and DL Beveridge.

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

270 Hrs.
(18 hrs/week)

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. $VO(acac)_2$

ii. $TiO(C_9H_8NO)_2.2H_2O$

iii. cis-$K[Cr(C_2O_4)_2(H_2O)_2]$

iv. $Na[Cr(NH_3)_2(SCN)_4]$

v. $Mn(acac)_3$

vi. $K_3[Fe(C_2O_4)_3]$

vii. PrussianBlue,Turnbull'sBlue.

viii. $Co(NH_3)_6][Co(NO_2)_6]$.

ix. cis-$[Co(trien)(NO_2)_2]Cl.H_2O$

x. $Hg[Co(SCN)_4]$

xi. $[Co(Py)_2Cl_2]$

xii. $[Ni(NH_3)_6]Cl_2$

xiii. $Ni(DMG)_2$

xiv. $[Cu(NH_3)_4]SO_4.H_2O$

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 ß-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,pipetteandstandardflask.

B. **Adsorption:**

i. To study surface tension-concentration relationship for solutions (Gibbsequation).

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, Adward 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. - Xth Semester

(Course Content)

CHY - 1001: Photochemistry/ Solid State

1. **Photochemistry**

a) Photochemical Reactions. Determination of Reaction Mechanism

b) Photochemistry of Alkenes

c) Photochemistry of Carbonyl Compounds

d) Photochemistry of Aromatic Compounds Miscellaneous Photochemical Reactions

2. **Solid State Chemistry**

a) Solid State Reactions Crystal Defects and Non-Stoichiometry

b) Electronic Properties and Band Theory

c) Organic Solids

CHY - 1002: Environmental Chemistry

1. Environment
2. Hydrosphere
3. Soils
4. Atmosphere
5. Industrial Pollution
6. 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, actionometry. — 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, β-γ Unsaturated and α-β unsaturated compounds, cyclohexadienones, intermolecular cycloaddition reactions-dimerisation and oxectane 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- Schotty defects and Frenkel defects, thermodynamics of Schotky 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. **15**

15

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,

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, biochemicaloxygen 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 Eastem.
iv. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastem
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 load compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR). factors affecting bloactivity, 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_{50}, ED_{50} (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,

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 oxyprenolol.

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, econozole, 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, benzodiazipines, 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, ethosuximde, 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. Wiey-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 Giman'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 stools, 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**

Mesmorphic behaviour, thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases: smectic nomatic 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

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:

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. 8

7. High Tc Materials: 10

Defect perovskites, high Tc 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 mutti gap structures in high Tc materials, applications of high Tc materials.

8. Materials for Solid State Devices:

Rectifiers, transistors, capacitors -IV-V compounds, low-dimensional quantum structures: optical properties. 3

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 Verleg.

CHN-10033: Organic Synthesis II **60 Hrs.**

1) **Disconnection Approach:** **30**

An introduction to synthons and synthetic equivalents, disconnectionapproach, 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, regioselectiviity. 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.

Penzilli.n, 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 inito 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 lonisation 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

Theory of isotope effects. Primary and secondary kinetic isotope effects. Heavy atom isotope effects. Tunneling effect. Solvent effects.

4. Structural Effects on Reactivity: 6

Linear free energy relationships (LFER). The Hammett equation, substituent constants, theories of substituent effects. Interpretation of a-values, Reaction constant p. Deviations from Hammett equation. Dual-parameter correlations, inductive substituent constant. The Taft model, ar- and de-scales.

5. Solvation and Solvent Effects: 6

Qualitative understanding of solvent-solute effects on reactivity. Thermodynamic measure of solvation. Effects of solvation on reaction rates and equilibria. Various empirical indexes of solvation based on physical properties, solvent-sensitive reaction rates, spectroscopic properties and scales for specific solvation. Use of solvation scales in mechanistic studies. Solvent effects from the curve-crossing model.

6. Acids, Bases, Electrophiles, Nucleophiles and Catalysis: 6

Acid-base dissociation. Electronic and structural effects, acidity and basicity. Acidity functions and their applications. Hard and soft acids and bases. Nucleophilicity scales. Nucleofugacity. The a-effect. Ambivalent nucleophiles. Acid-base catalysis specific and general catalysis. Bronsted catalysis. Nucleophilic and electrophilic catalysis, Catalysis by non-covalent binding-micellar catalysis.

7. Steric and Conformational Properties: 6

Various type of steric strain and their influence on reactivity. Steric acceleration, Molecular measurements of steric elfects upon rates. Steric LFER. Conformational barrier to bond rotation-spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein-Holness and Curtin-Hammett principle.

8. Nucleophilic and Electrophilic Reactivity: 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, Elecrophilic reactivity, general mechanism, Kinetic S2-Ar reaction. Structural effects on rates and selectivity Curve-crossing approach to 6

electrophilic reactivity.

9. Radical and Pericyclic Reactivity:

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

10. Supramolecular Chemistry: 5

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 enorgy 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.

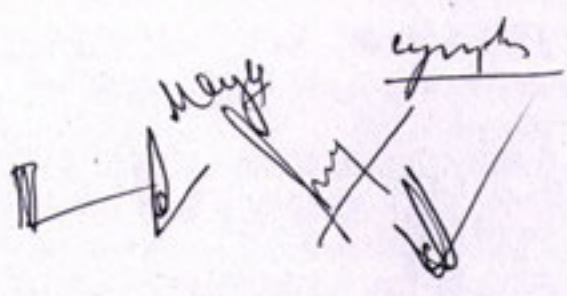
iii. Mechanism and Theory in Organic Chemistry, T. H. Lowry and K. C.Richardson, and Row

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

60 Hrs.

CHY-10041: Polymer Chemistry

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. Numbor, weight and viscocity average molecular weights. Polydispersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End-group, viscocity, 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 Tm-melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, Tg-Relationship between Tm and Tg. 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 Commerical 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-Eastem.
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 formulao, 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 tumes-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

Structura, 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 excred 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-exciplex 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 phenonthroine complexes). Illustration of reducing and oxidising character of Ruthenium (pyridal complex, comparison with Felblpyls: role of spin-orbit coupling-fe 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, AW Adamson and P.D. Fischauer, Wiley

ii. Inorganic Photochemistry, J. Chem. Educ, vol 00, no. 10, 1003

iii. Progress in trorganic Chemistry, vol. 30, ed. 5.J. Lippan Wiley.

iv. Coordination Chem, Revs 1981, vol 39, 121, 131, 1975 15 321, 1000, 97, 313 5.

v. Premistry of Coordination Compounds, V. Batra and V. Caras, Academic Press 6.

vi. Elements of inorganic Photochemistry G. J. Feraud Whey

CHY-10044: Heterocyclic Chemistry **60 Hrs**

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 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 quinolizinium and benzopyrylium salts, coumarins and

chromones

9. Six-Membered Heterocycles with Two or More Heteroatoms 5

Synthesis and reactions of diazines, triazines, tetrazinesand thiazines

10. Seven and Large Membered Heterocycles 5

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

11. Heterocyclic System Containing P, As, Sb and B 10

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 S 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, Chapmanand Hall

iv. Heterocyclic Chemistry,T.L Gilchrist,Longman Scietific Techinal

v. Contemporary Heterocyclic Chemistry, G. A. Newkome and W. W.Paudler, Wiley-Inter Science

vi. An Introduction to the. Heterocyclic Compounds, A. M. Acheson,JohnWiley

vii. Comprehensive Heterocyclic Chemistry, A. A. Katritzky and C. W. Rees. ads. Pergamon Press

CHY-1005: Practical (Instrumental methods of Analysis and Organic Synthesis) **270 Hrs.** (18 hrs/week)

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-

CC

(i) Photochemical reaction

Benzophenone → Benzpinacol-Benzpinacolone

(ii) Beckmann rearrangement: Benzanilide from benzene

Benzene Benzophenone Benzophenone oxime →Benzanilide

(iii) Benzilic acid rearrangement: Benzilic acid from benzoin

Benzoin Benzil→ 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