Choice Based Credit System (CBCS)

JAMIA MILLIA ISLAMIA

(A CENTRAL UNIVERSITY)

FACULTY OF NATURAL SCIENCES

M.Sc. CHEMISTRY

(Effective from Academic Year 2022-23)

SYLLABUS OF COURSES TO BE OFFERED

Core, Elective, Skill and Ability Enhancement Courses

Brief Description about the Course

MSc. Chemistry course work is designed for students, to enhance their practical skills, and knowledge in various disciplines offered by the Department: Organic, Inorganic, Physical and Materials Chemistry. The curriculum is prepared with the view to help students secure jobs in different chemical industries/teaching institutes or secure PhD positions in any reputed national/international University/Institute.

The programme consists of 4 semesters, worth a total of 88 credits, delivered in 24 months including a substantial in-house project work carried out in the last semester.

The core objective is to train students with essential theoretical and practical skills in the synthesis, characterization and processing techniques with reference to Organic, Inorganic, Physical and Materials Chemistry. An in-depth experience of research is provided through individual Masters Project work.

As per the Choice Based Credit System (CBCS), the breakup of the papers (core, elective and ability enhancement) and Lab wok offered to the students in every semester is provided in the course outline table along with the credit details. In all semester, the Core papers are of 3 credits each (100 marks) consisting of university exam (UE) (60 marks) and internal assessment (IA) (40 marks). During the first two semesters, the practical course carries one credit (50 marks) while in the 3rd and 4th semester, it carries 4 credits. Elective, ability and skill enhancement papers carry 4 credits each. The in-house project work of 3 credits (150 marks) and Educational Tour of 1 credit (50 marks) is offered in MSc 4th semester. The details of the project work are given in the last page of the syllabus.

M. Sc. Programme
Proposed Semester-wise Number of Papers & Credits under the Choice Base Credit System (CBCS)

Semester	Core Courses	Choice Based Courses (Elective)	Skill Enhance-ment Courses (SEC)	Ability Enhance-ment Compulsory Course (AECC)	Total papers	Credits
I	3°/4	1	-	-	3/4+1=4/5	16/20
II	3°/4	1	1	-	3/4+1+1=5/6	20/24
III	4°/4	1	-	1	4+1+1=6	24
IV	4°/4	1	-	-	4+1=5	20
No. of Papers	14° / 16	4	1	1	20/24	-
Total Credits	**4x14=56*° 4x16=64***	**4x4=16**	**4x1=4**	**4x1=4**	-	**80/88**

*Includes a Project work of 4 Credits
°Papers for those programmes which do not have practicals

Course Outline

SEMESTER-I

Paper/ Practical	Paper No	Paper Code	Paper Title	Total Credits (Marks)
Theory (Core)	I	MCH-101	Inorganic Chemistry-I	03 (100)
Practical (Core)		MCH-101L	Inorganic Chemistry Practical-I	01 (50)
Theory (Core)	II	MCH-102	Elements of Materials Chemistry –I	03 (100)
Practical (Core)		MCH-102L	Elements of Materials Chemistry Practical-I	01 (50)
Theory (Core)	III	MCH-103	Stereochemistry and Reactive Intermediates	03 (100)
Practical (Core)		MCH-103L	Organic Chemistry Practical-I	01 (50)
Theory (Core)	IV	MCH-104	Thermodynamics & Statistical Thermodynamics	03 (100)
Practical (Core)		MCH-104L	Physical Chemistry Practical-I	01 (50)
Theory (Elective)	V	MCH-105	Group Theory and Spectroscopy-I	04(100)
TOTAL CREDITS (3 x 4T+ 4 x 1P + 4) = 20			TOTAL MARKS =700	

SEMESTER-II

Theory (Core)	VI	MCH-201	Inorganic Chemistry-II	03 (100)
Practical (Core)		MCH-201L	Inorganic Chemistry Practical -II	01 (50)
Theory (Core)	VII	MCH-202	Elements of Materials Chemistry-II	03 (100)
Practical (Core)		MCH-202L	Elements of Materials Chemistry Practical-II	01 (50)
Theory (Core)	VIII	MCH-203	Pericyclic Reactions andPhotochemistry	03 (100)
Practical (Core)		MCH-203L	Organic Chemistry Practical-II	01 (50)
Theory (Core)	IX	MCH-204	Macromolecules & Surface Chemistry	03 (100)
Practical (Core)		MCH-204L	Physical Chemistry Practical -II	01 (50)
Theory (Elective)	X	MCH-205	Group Theory & Spectroscopy-II	04 (100)
Theory(Skill Enhancement)	XI	MCH-206	Mathematical & Computational Methods in Chemistry	04 (100)
TOTAL CREDITS (3 x 4T+ 4 x 1P+ 2 x 4) = 24			TOTAL MARKS = 800	

INORGANIC CHEMISTRY

SEMESTER-III

Theory (Core)	**XII (i)**	**MCH-301**	**NMR Spectroscopy and Lanthanide Shift Reagents**	**03 (100)**
Theory (Core)	**XIII (i)**	**MCH-302**	**Inorganic Reaction Mechanisms**	**03 (100)**
Theory (Core)	**XIV (i)**	**MCH-303**	**Organometallic Chemistry-I**	**03 (100)**
Theory (Core)	**XV (i)**	**MCH-304**	**Bio-inorganic Chemistry – I**	**03 (100)**
Theory (Elective)	**XVI**	**MCH-317**	**Chemistry of Synthetic and Natural Materials-I**	**04 (100)**
Theory (Ability Enhancement)	**XVII**	**MCH-318**	**Environmental and Green Chemistry**	**04 (100)**
Practical		**MCHIL**	**Inorganic Chemistry Practical –III**	**04 (100)**

TOTAL CREDITS (3 x 4T+ 4 x 1P+ 2 x 4) = 24 TOTAL MARKS = 700

SEMESTER-IV

Theory (Core)	**XVIII (i)**	**MCH-401**	**Chemical Applications of Group Theory**	**03 (100)**
Theory (Core)	**XIX (i)**	**MCH-402**	**Stereochemistry and Metal Ion Catalysis**	**03 (100)**
Theory (Core)	**XX(i)**	**MCH-403**	**Organometallic Chemistry-II**	**03 (100)**
Theory (Core)	**XXI(i)**	**MCH-404**	**Bio-inorganic Chemistry – II**	**03 (100)**
Theory (Elective)	**XXII**	**MCH-417**	**Chemistry of Synthetic and Natural Materials-II**	**04 (100)**
Project Work				**03 (150)**
Educational Tour (Approved by AC & EC) [25 Marks of visit + 25 educational tour report]				**01 (50)**

TOTAL CREDITS (3 x 4T+ 2 x 4) = 20 TOTAL MARKS = 700

MATERIALS CHEMISTRY

SEMESTER-III

Theory (Core)	**XII (ii)**	**MCH-305**	**Conventional Ceramics**	**03 (100)**
Theory (Core)	**XIII (ii)**	**MCH-306**	**Basic Concepts of Crystallography& Crystal Structures**	**03 (100)**
Theory (Core)	**XIV (ii)**	**MCH-307**	**Polymer Chemistry &Technology**	**03 (100)**
Theory (Core)	**XV (ii)**	**MCH-308**	**Chemistry of Advanced Materials**	**03 (100)**
Theory (Elective)	**XVI**	**MCH-317**	**Chemistry of Synthetic andNatural Materials-I**	**04 (100)**
Theory (Ability Enhancement)	**XVII**	**MCH-318**	**Environmental and GreenChemistry**	**04 (100)**
Practical		**MCHML**	**Materials Chemistry Practical-III**	**04 (100)**

TOTAL CREDITS (3 x 4T+ 4 x 1P+ 2 X 4) = 24 TOTAL MARKS = 700

SEMESTER-IV

Theory (Core)	**XVIII (ii)**	**MCH-405**	**Technical Ceramics**	**03 (100)**
Theory (Core)	**XIX (ii)**	**MCH-406**	**Processing and characterization of Crystal Structures**	**03 (100)**
Theory (Core)	**XX(ii)**	**MCH-407**	**Polymer Technology, Processing and Specialty Polymers**	**03 (100)**
Theory (Core)	**XXI(ii)**	**MCH-408**	**Properties of Materials**	**03 (100)**
Theory (Elective)	**XXII**	**MCH-417**	**Chemistry of Synthetic and Natural Materials-II**	**04 (100)**
Project Work				**03 (150)**
Educational Tour (Approved by AC & EC) [25 Marks of visit + 25 educational tour report]				**01 (50)**

TOTAL CREDITS (3 x 4T+ 2 x 4) = 20 TOTAL MARKS = 700

ORGANIC CHEMISTRY

SEMESTER-III

Theory (Core)	**XII (iii)**	**MCH-309**	**Methods in Organic Synthesis**	**03 (100)**
Theory (Core)	**XIII (iii)**	**MCH-310**	**Advance Tools In Organic Synthesis**	**03 (100)**
Theory (Core)	**XIV (iii)**	**MCH-311**	**Reagents and Organic Synthesis**	**03 (100)**
Theory (Core)	**XV (iii)**	**MCH-312**	**Chemistry of Heterocyclic Compounds**	**03 (100)**
Theory Elective	**XVI**	**MCH-317**	**Chemistry of Synthetic and Natural Materials-I**	**04 (100)**
Theory Ability Enhancement	**XVII**	**MCH-318**	**Environmental and GreenChemistry**	**04 (100)**
Practical		**MCHOL**	**Organic Chemistry Practical -III**	**04 (100)**

TOTAL CREDITS (3 x 4T+ 4 x 1P+ 2 x 4) = 24 TOTAL MARKS = 700

SEMESTER – IV

Theory (Core)	**XVIII (iii)**	**MCH-409**	**Medicinal Chemistry and Biomolecules**	**03 (100)**
Theory (Core)	**XIX (iii)**	**MCH-410**	**Advanced Methods in Organic synthesis**	**03 (100)**
Theory (Core)	**XX(iii)**	**MCH-411**	**Chemistry of Natural Products**	**03 (100)**
Theory (Core)	**XXI(iii)**	**MCH-412**	**Applications of Spectroscopy**	**03 (100)**
Theory (Elective)	**XXII**	**MCH-417**	**Chemistry of Synthetic and Natural Materials-II**	**04 (100)**
Project Work				**03 (150)**
Educational Tour (Approved by AC & EC) [25 Marks of visit + 25 educational tour report]				**01 (50)**

TOTAL CREDITS (3 x 4T+ 2 x 4) = 20 TOTAL MARKS = 700

PHYSICAL CHEMISTRY

SEMESTER-III

Theory (Core)	**XII (iv)**	**MCH-313**	**Advanced Statistical Mechanics**	**03 (100)**
Theory (Core)	**XIII (iv)**	**MCH-314**	**Advanced Solid State Chemistry**	**03 (100)**
Theory (Core)	**XIV (iv)**	**MCH-315**	**Chemical Kinetics**	**03 (100)**
Theory (Core)	**XV (iv)**	**MCH-316**	**Quantum Chemistry**	**03 (100)**
Theory Elective	**XVI**	**MCH-317**	**Chemistry of Synthetic and Natural Materials-I**	**04 (100)**
Theory Ability Enhancement	**XVII**	**MCH-318**	**Environmental and Green Chemistry**	**04 (100)**
Practical		**MCHPL**	**Physical Chemistry Practical -III**	**04 (100)**

TOTAL CREDITS (3 x 4T+ 4 x 1P + 2 x 4) = 24 TOTAL MARKS = 700

SEMESTER-IV

Theory (Core)	**XVIII (iv)**	**MCH-413**	**Advance Molecular spectroscopy**	**03 (100)**
Theory (Core)	**XIX (iv)**	**MCH-414**	**Nano Chemistry**	**03 (100)**
Theory (Core)	**XX (iv)**	**MCH-415**	**Advance Physical Chemistry**	**03 (100)**
Theory (Core)	**XXI(iv)**	**MCH-416**	**Electrochemistry**	**03 (100)**
Theory Elective	**XXII**	**MCH-417**	**Chemistry of Synthetic and Natural Materials-II**	**04 (100)**
Project Work				**03 (150)**
Educational Tour (Approved by AC & EC) [25 Marks of visit + 25 educational tour report]				**01 (50)**

TOTAL CREDITS (3 x 4T+ 2 x 4) = 20 TOTAL MARKS = 700

M.Sc. CHEMISTRY
SEMESTER - I

MCH-101 Paper No: I	INORGANIC CHEMISTRY-I	Theory (Marks)		Total Credits (Marks)
		U.E. (60)	I.A. (40)	03 (100)

Objective: Introduction metal ligand equilibria, non-aqueous solvents and to help students understand the basics of Inorganic Materials

Unit I: 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. **12 L**

Unit II: Non–Aqueous Solvents

Role of Solvents in chemical reactions, physical properties of a solvent, types of solvent andtheir general characteristics, reactions in non-aqueous solvents with reference to liquid ammonia and liquid SO_2. **12 L**

Unit III: Magnetic Properties of Transition Metal Complexes

Magnetic properties of transition metal complexes and lanthanides, spin-orbit coupling and susceptibility of transition metal ions and rare earths; magnetic moments of metal complexes with crystal field terms of A, E and T symmetry, T.I.P., intra-molecular effects, anti-ferromagnetism and ferromagnetism of metal complexes, super paramagnetism. High and low spin equilibria, anamolous magnetic moments, magnetic exchange coupling and spin Crossover. **14 L**

Unit IV: Inorganic Materials

Introduction to the solid state, metallic bond, band theory (zone model, brillouin zones, limitation of zone model): defects in solids, *p*-type and *n*-type, inorganic semiconductors (use in transistors, IC etc.), electrical, optical, magnetic and thermal properties of inorganic materials, superconductors, with special emphasis on the synthesis and structure of high temperature superconductors. **12 L**

Essential Reading

1. Inczedy, J. *Analytical applications of complex equilibria* Halsted Press: New York, NY (1976)..
2. Hartley, F. R., Burgess, C. & Alcock, R. M. *Solution Equilibria* Prentice-Hall: Europe (1980).
3. Ringbom, A. *Complexation in Analytical Chemistry* Wiley: New York (1963).
4. Non-aqueous Solution Chemistry by H.H. Sisler
5. Magnetochemistry by R.L. Carlin.

Suggested Reading

1. Mabbs, F. E. & Machin, D. J. *Magnetism and Transition Metal Complexes* Chapman and Hall:U.K.(1973).
2. Keer, H.V. *Principles of the solid state* Wiley Eastern Ltd.: New Delhi (1993).
3. West, A.R. *Solid State Chemistry and its Applications* John Wiley & Sons (1987).
4. Cheetham, A. K. & Day, P., Eds. *Solid State Chemistry Techniques* Clarendon Press, Oxford (1087).

M.Sc. CHEMISTRY
SEMESTER - I

Practical Course Work

MCH-101L	INORGANIC CHEMISTRY PRACTICAL -I	Practical (Marks)		Total Credits (Marks)
		U.E. (25)	I.A.(25)	01 (50)

S. No. **EXPERIMENT**

1. **Synthesis and Characterization of Complexes**
   Preparation of the following inorganic compounds and their studies by IR, electronic spectra, Mossbauer and ESR spectra
   (I) $VO(acac)_2$
   (II) *Cis*-$K[Cr(C_2O_4)_2(H_2O)_2$
   (III) $Na[Cr(NH_3)_2(SCN)_4]$
   (IV) $K_3[Fe(C_2O_4)_3]$

2. **Quantitative Analysis**
   Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe, Ba-Cu etc. involving volumetric and gravimetric methods.

3. **Spectrophotometric Determinations**
   3.1 Ni by extractive spectrophotometric method.
   3.2 Fe by Job's method of continuous variations
   3.3 Fe in vitamin tablets
   3.4 Nitrite in water in colorimetric method

Reference Books:

1. Experimental Inorganic Chemistry by W.G. Palmer, Cambridge.
2. Inorganic Synthesis, MC Graw Hill.
3. Handbook of Preparative Inorganic chemistry Vol. I and II, Academic press.
4. Standard methods of chemical analysis by W.W. Scaff, Technical Press.
5. Vogel's Qualitative Inorganic Analysis (revised), Orient Longman.
6. Vogel's textbook of quantitative Inorganic Analysis (revised).

M.Sc. CHEMISTRY
SEMESTER - I

MCH-102 Paper No: II	ELEMENTS OF MATERIALSCHEMISTRY-I	Theory (Marks)		Total Credits (Marks)
		U.E.(60)	I.A. (40)	03 (100)

Objective: Introduction to basic types of Materials to help students understand the Structure-Property relationship of various kinds of Materials

Unit I: Glasses **8 L**

General features, Fabrication of glass, Factors effecting glass formation: Viscosity; Electronegativity; bond types; Theories of glass formation: Zachariasen's Rule, Sun and Rawson Criteria; Thermodynamics of Glass Formation; Methods of Glass Formation; Various Types of Glasses and Their Properties: Pyrex Glass; Vycor Glass; Phosphate Glasses, Borate glasses, Chalcogenide Glasses

Unit II: Multiphase Materials **12 L**

Solid solutions; Interstitial and Substitutional solid solutions; Complex Solid Solutions; Intermetallic Compounds; Condensed Phase Rule; One Component System: Si and Fe; Binary isomorphous system: Cu-Ni, Au-Cu, Hume Rothery; Solid Solubility Rule; Liver Rule; Invarient Phase Equilibrium; Eutetic Formation (Pb-Sn); Peritectic Formation: Fe-Ni, Fe-C Phase Diagram; Phase Transformation : Fe-C alloys, Ferrous and non-ferrous alloys

Unit III: Polymeric Materials **14 L**

Definition. General Characteristics and Examples of Polymers; Classification of Polymers; Methods of Polymerization: General Characteristics of Chain Growth Polymerization; Alkene Polymerization by Free Radical, Cationic and Anionic Initiators Mass Polymerization Techniques: Bulk and Solution Methods General Characteristics of Step Growth Polymerization; Synthesis of Polymers by Step Growth Polymerization: Polyesters, Polyamides, Polycarbonates, Polysulphones, Polyphenyl oxides and Polysiloxanes, Copolymers, Copolymer Equation and its Application, Monomer Reactivity Ratios

Unit IV: Nanomaterials

Nano-scale Regime; Types of Nanomaterials: Nanoparticle, Nanoporous; Gas phase Nanoparticles; Condensed Phase Nanoparticles; Inorganic Nano Particles; Methods of Preparation: Bottom up; Top down; Reduction methods; Sol-Gel Methods; Co-Precipitation Method; Zeolite Method; Emulsion Method; Properties of Nanoparticles: Physical, Mechanical, Chemical, Magnetic, Optical and electronic properties **14 L**

Essential Reading:

1. Introduction to Solid State Chemistry A.R.West
2. Materials Science and Engineering: An Introduction, W.D. Callister, Wiley
3. Text Book of Polymer Science by F. W. Billmeyer
4. Introduction to Polymers by R. J. Young and P. A. Lovell

M.Sc. CHEMISTRY
SEMESTER - I

Suggested Reading:

1. Introduction to Materials Chemistry by Harry R. Allcock.
2. Inorganic Materials Chemistry by Book by Mark Weller.
3. Principles of solid state, H. V. Keer, Wiley Eastern.
4. Chemistry of Advanced Materials by Leonard V. Interrante and M. J. Hampden-Smith
5. Polymer Chemistry by G. Challa.

M.Sc. CHEMISTRY
SEMESTER - I

Practical Course Work

MCH-102L	ELEMENTS OF MATERIALS CHEMISTRY PRACTICAL-I	Practical (Marks)		Total Credits (Marks)
		UE (25)	IA (25)	01 (50)

S.No	EXPERIMENT
1.	**Analysis of steel sample**: 1.1 To determine the percentage of manganese in the given sample of steel 1.2 To determine the percentage of phosphorous in the given sample of steel 1.3 To determine the percentage of sulphur in the given sample of plain carbon steel 1.4 To determine the percentage of silicon in the given sample of plain carbon steel
2.	**Analysis of brass sample:** 2.1 To determine the percentage of tin in the given sample of brass 2.2 To determine the percentage of lead in the given sample of brass 2.3 To determine the percentage of copper in the given sample of brass 2.4 To determine the percentage of zinc in the given sample of brass
3.	Synthesis of polymers: 3.1 To prepare polystyrene by bulk polymerization method and report the yield and solubility 3.2 To determine the Molecular Weight of the prepared polystyrene by viscometry 3.3 To determine the Molecular Weight of commercial polystyrene by viscometry and compare the molecular weights of the prepared and commercial polystyrene.

Reference books:

1. Laboratory manual prepared by the Teacher–in-Charge

M.Sc. CHEMISTRY
SEMESTER - I

MCH-103 Paper No: III	STEREOCHEMISTRY & REACTIVE INTERMEDIATES	Theory (Marks)		Total Credits (Marks)
		U.E.(60)	I.A(40)	03 (100)

Objective: The unit comprises of Isomerism, Aromaticity, Conformational Analysis and ReactiveIntermediates help students understand the basics of advance Organic Reactions

Unit I Configurational Isomerism **8 L**

Stereoisomerism: classification, optical activity and chirality resolution of racemic mixture, molecules with one, two or more chiral centres; Fischer's projection formula, relative and absolute configurations, D L, R S, and E Z system of naming. Stereochemistry due to the presence of perpendicular dissymmetric planes in allenes, spiranes, biphenyls and binaphthols. Chirality due to helical shape and chiral due to chiral plane. Optical purity, % enantiomeric excess (ee), enantiotopic and diastereotopic atoms groups and faces. The FelkinAnh and Cornforth model, Cram's and Prelog's rules.

12 L

Unit II: Aromaticity and Principles of Reactivity

Huckel's rule and Craig's rule of aromaticity, benzoid and non-benzoid aromatic systems; annulenes, fulvenes, fulvalenes, tropones, azulene, squaric acid, pentalene and heptalene anti-aromaticity, homo-aromaticity and Frost diagrams and consequences of aromaticity. Transition state theory, Hammond postulate, Marcus relation-methods of elucidating reaction mechanism-kinetic and non-kinetic methods-stereo chemical evidences –cross over experiments- Isotopic effects-linear free energy relation-Hammett equation-significance of σ and ρ, Taft equation, Swain-Scott equation-Winstein-Grunwald equation

Unit III: Conformational Analysis **08 L**

Conformation in open chain systems, conformational analysis of cyclopentane, cyclohexane, decalins, sugars, steroids, and rings containing sp2 hybridized 2 carbon atoms. Baeyer's strain theory of cyclic compounds, and, effect of conformation on reactivity.

14 L

Unit IV: Reactive Intermediates

Carbocations: Classical and Nonclassical carbocations, neighbouring group participation, stability and reactivity of bridge-head carbocations. Bredts rule, Carbanions: Stability and structure, the structure of organometallic compounds generation and fate, ambident ions and their general reactions; HSAB principle and its applications. Carbon free radicals: Stability and structure, generation and fate of free radicals, captodative effects; radical-ions.Generation, structure and reactions of carbenes, nitrenes, benzynes intermediates

Essential Reading

1. Advanced Organic Chemistry; Jerry March, Fourth edition, Wiley & Sons, (2005).
2. Organic Chemistry; Paula Yurkanis Bruice, Third edition, Pearson, (2004).
3. Advanced Organic Chemistry; Francis A. Carey and Richard J. Sundberg,

Suggested Reading

1. Organic Reactions, Stereochemistry and Mechanisms; P.S. Kalsi, Fourth edition, New Age International Publishers, (2006).
2. Eliel, E. L. Stereochemistry of Carbon Compounds Textbook Publishers, 2003.
3. Bruckner, R. Advanced Organic Chemistry Elsevier (2002).

M.Sc. CHEMISTRY
SEMESTER - I

Practical Course Work

MCH-103L	ORGANIC CHEMISTRY PRACTICAL-I	Practical (Marks)		Total Credits (Marks)
		UE (25)	IA (25)	01 (50)

S.No	EXPERIMENT
1.	Purification techniques (Demonstrations). Purification of solvents and reagents using techniques like crystallization, sublimation, fractional distillation, vacuum distillation, drying and storage of solvents, thin layer chromatography and column chromatography etc.
2.	Separation of a binary mixture of organic compounds and identification of the separated components by systematic qualitative organic analysis
3.	Separation of a ternary mixture of organic compounds and identification of the separated components by systematic qualitative organic analysis
4.	Preparations of the following compounds 4.1 4-Iodonitrobenzene 4.2 Hippuricacid 4.3 Sorbicacid 4.4 Methylorange 4.5 Flourescein 4.6 Oil of wintergreen 4.7 Benzamidazole

Reference Books

1. Comprehensive Practical Organic Chemistry by V.K.Ahluwalia
2. Monograph on Green Chemistry Laboratory Experiments by Green Chemistry TaskForce Committee,DST.
3. Advanced practical (organic chemistry) by N. K.Vishnoi.

M.Sc. CHEMISTRY
SEMESTER - I

MCH-104 Paper No: IV	THERMODYNAMICS & STATISTICAL THERMODYNAMICS	Theory (Marks)		Total Credits (Marks)
		U.E. (60)	I.A. (40)	03 (100)

Objective: The unit deals with the advance concepts of thermodynamics

Unit I: Equilibrium Thermodynamics

Partial molar quantities and their physical significances, Determinations of the partial molar quantities, Chemical potential and other thermodynamic functions, Variation of chemical potential with temperature and pressure, Chemical potential for Ideal gas mixture, Thermodynamic Functions of Mixing, Concepts of Fugacity, and its determination. Gibbs Duhem Margules equation and its applications. **09 L**

Unit II: Non Equilibrium Thermodynamics

Thermodynamic criteria for non-equilibrium states, Basic Postulates and Methodology, Onsager's Theory, Phenomenological Laws and Equations, Transformations of the generalized fluxes and forces, Microscopic Reversibility and Onsager's Reciprocal Relations, Entropy Production and entropy flow, Theorem of Minimum Entropy Production, Electro-kinetic Phenomena. **12 L**

Unit III: Statistical Thermodynamics-I

Idea of microstates and macrostates, Concept of distribution-Binomial & multinomial distribution for non-degenerate and degenerate systems, Thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical and other ensembles, Statistical mechanics for systems of independent particles and its importance in chemistry. Types of statistics: Boltzmann, Bose-Einstein and Fermi-Dirac statistics. Thermodynamic probability (W) for the three types of statistics. Derivation of distribution laws (most probable distribution) for the three types of statistics. Lagrange's undetermined multipliers. Stirling's approximation, Molecular partition function and its importance. Assembly partition function. **12 L**

Unit IV: Statistical Thermodynamics-II

Applications to ideal gases: The molecular partition function and its factorization. Evaluation of translational, rotational and vibrational partition functions for monatomic, diatomic and polyatomic gases. The electronic and nuclear partition functions. Calculation of thermodynamic properties of ideal gases in terms of partition function. Statistical definition of entropy. Ortho- and para-hydrogen, statistical weights of ortho and para states, symmetry number. Calculation of equilibrium constants of gaseous solutions in terms of partition function, perfect gas mixtures. Einstein theory and Debye theory of heat capacities of monatomic solids. Third law of thermodynamics, Residual entropy. **12 L**

M.Sc. CHEMISTRY
SEMESTER - I

Essential Reading

1. An Introduction to Chemical Thermodynamics, R. P. Rastogi and R. R. Mishra, VikasPublishing House Pvt. Ltd.
2. Physical Chemistry, P. W. Atkins, ELBS.
3. Statistical Thermodynamics (Hardback) By (author) M.C. Gupta, Publisher: New AgeInternational.
4. Thermodynamics, J. Rajaram and J.C. Kuriacose, Educational Publishers.
5. Statistical Mechanics, Donald A. McQuarrie, Viva Books Pvt. Ltd. New Delhi, 2003 (530.13MCQ 270916)

Suggested Reading

1. Thermodynamics, R. C. Srivastava, Subit K. Saha, Abhay K. Jain, Prentice Hall of India, Pvt.Ltd.
2. Statistical Physics (Part) Course of Theoretical Physics, Vol. 5, L. D. Landau and E. M. Lifshitz,Pergamon Press London.
3. Physical Chemistry, T. Engel and P. Reid, Pearson Education and Dorling Kindersley (India)2006.
4. Elements of Statistical Thermodynamics (2nd Edition), Leonard K. Nash, Addison Wesley, 1974.(541.369 NAS X639)
5. Physical Chemistry, *Statistical Mechanics*, Horia Metiu, Taylor & Francis, 2006 (530.13 MET276461)
6. Statistical Thermodynamics, B.J. McClelland, Chapman and Hall & Science Paperbacks,London, 1973 (536.7 MCC 37251)

M.Sc. CHEMISTRY
SEMESTER - I

Practical Course Work

MCH-104L	PHYSICAL CHEMISTRY PRACTICAL-I	Practical (Marks)		Total Credits (Marks)
		UE (25)	IA (25)	01 (50)

S.No	EXPERIMENT
1.	Determine the percentage composition of a liquid mixture by viscosity method.
2.	Determine the radius of sucrose molecule by viscosity method.
3.	Determine molar surface energy of ethyl alcohol by surface tension.
4.	To find out composition of a solution by surface tension measurement.
5.	Find out molar surface area as a function of concentration for n– propyl alcohol and nbutyl alcohol over water.
6.	Verify the law of refraction for mixtures, using glycerol and water.
7.	Determine the formation of compounds between two liquids in the mixture.
8.	Study the saponification of ethyl acetate by sodium hydroxide solution.
9.	Compare the strengths of hydrochloric acid and sulphuric acid by studying the rate of hydrolysis of methyl acetate.
10.	Determine the specific reaction rate of the potassium persulphate iodide reaction by initial rate method.
11.	Study of the kinetics of the iodination of acetone in the presence of acid by the initial rate method.
12.	Study the adsorption of oxalic acid on charcoal.
13.	Determine the heat of neutralization of hydrochloric acid and sodium hydroxide.
14.	Determine the heats of reaction for the reactions: (i) $CO_3^{2-} + H_2O \rightarrow HCO_3^- + OH^-$ (ii) $HC_2O_4^- + H_2O \rightarrow H_2C_2O_4 + OH^-$
15.	Find out the dimerization constant of benzoic acid in benzene by titration method.
16.	Construct the phase diagram of water-ethanol-benzene system
17.	Find out the molar mass of succinic acid by partition method

M.Sc. CHEMISTRY
SEMESTER - I

MCH-105 Paper No: V	GROUP THEORY AND SPECTROSCOPY	Theory (Marks)		Total Credits (Marks)
		UE(60)	IA(40)	04 (100)

Objective: The unit deals with the basic concepts of group theory and electronic spectroscopy

Unit I Symmetry and Group Theory -I **12 L**

Symmetry elements operation. Definition of a symmetry operation. Definition of a symmetry element. Symmetry planes and reflection. The inversion centre. Proper axes and proper rotations. Improper axes and improper rotations. Identity. Products and symmetry operations. Defining properties of a group. Abelian group. Symmetry operations as group elements (Multiplication table). Symmetry point group (Schoenflies notations). Classes of symmetry, operations. Equivalent symmetry elements and atoms.

Unit-II: Symmetry and Group Theory-II **12 L**

Character tables for C_{2V} and C_{3V} point groups (Construction not required). Representation reducible and irreducible, analysis of reducible representation. Simple Applications of the character table.

Unit- III: Electronic Spectroscopy fundamentals **10 L**

Atomic Spectroscopy: The energies of atomic orbitals; Hydrogen atom spectrum; Orbital and spin angular momenta, total angular momentum; the fine structure of hydrogen atom spectrum; the spectra of alkali metal atoms. The spectra of complex atoms: Singlet and triplet states; Spin-orbit coupling; Term Symbols and selection rules.

Unit- IV: Electronic Spectroscopy of Polyatomic Molecules **15 L**

Energy levels of molecular orbitals, vibronic transitions, vibrational progressions and geometry of excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Electronic spectra of transition metals Emission spectra: radiative and non-radiative decay, internal conversion, spectra of transition, metal complexes, charge-transfer spectra

Essential Reading

1. Modern Spectroscopy, J.M. Hollas, John Wiley & Sons(2004).
2. Applied Electronic Spectroscopy for Chemical Analysis Ed. H Windawi and F. L. Ho, Wiley Interscience.
3. NMR, NQR, EPR and Mössbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, Ellis Harwood
4. Physical Methods in Chemistry, R.S. Drago,Saunders.
5. Chemical Applications of Group Theory, F.A.Cotton.

Suggested Reading

1. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill(1962).
2. Basic Principles of Spectroscopy, R. Chang, McGraw Hill, N.Y.(1970)
3. Theory and Applications of UV Spectroscopy, H.H. Jaffe and M. Orchin, andIBH-Oxford.
4. Fundamentals of Molecular Spectroscopy, Fourth Edition, C.N. Banwell andE.M

M.Sc. CHEMISTRY
SEMESTER - II

MCH-201 Paper No: VI	INORGANIC CHEMISTRY-II	Theory (Marks)		Total Credits (Marks)
		U.E. (60)	I.A. (40)	03 (100)

Objective: The unit deals with the electronic spectra of transition metal complexes, stereochemistry, bonding of main group compounds and basics of Metal Clusters

Unit I: Electronic Spectra of Transition Metal Complexes
Spectroscopic ground states, correlation, crystal field theory and splitting in O*h*, T*d*, D*4h* and C*4v*systems, orgel and Tanabe-Sugano diagrams for transition metal complexes (d1 –d9), Calculation of Dq, B and β Parameters, charge transfer spectra, spectroscopic method for assignment of absolute configuration in-optically active metal chelate and their stereochemical information **12 L**

Unit II: Stereochemistry and Bonding in Main Group Compounds **10 L**
VSEPR, Walsh diagram (tri- and penta atomic molecules), dπ-pπ bonds, Bent rule andenergetic of hybridization, simple reactions of covalently bonded molecules.

Unit III: Unit III: Isopoly and Heteropoly Acids and Salts **08 L**
Isopolymolybdates, isopolytungstate, isopolyvanadates, heteropoly anions, organo heteropolyanions and Heteropoly blues.

Unit IV: Metal Clusters
Higher boranes, carboranes and metalloboranes, compounds with metal –metal multiplebonds metal carbonyls and halide clusters. **12 L**

Suggested Reading

1. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, Wiley, VCH, 1999.

2. D.F. Shriver and P.W. Atkins, Inorganic Chemistry, 3rd edn., Oxford University Press.

3. Inorganic Chemistry by G.L. Miessler and D.A. Tarr.

4. Inorganic Chemistry by Catherine E. Housecroft, A. G. Sharpe.

M.Sc. CHEMISTRY
SEMESTER - II

Practical Course work

MCH-201 L	INORGANICCHEMISTRY PRACTICAL -II	Practical (Marks)		Total Credits
		U.E. (25)	I.A. (25)	01 (50)

S. No **Experiment**

1. Qualitative Analysis
- 1.1 less common metal ions- Tl, Mo, Ti, Zr, Th, V and U (Two metal ions in cationic/anionicforms).
- 1.2 Insoluble- oxides, sulphates andhalides.

2. Chromatography ; Separation of cations and anions by
- 2.1 Paperchromatography.
- 2.2 Column chromatography- ion exchange.

3. Synthesis and Characterization of Complexes
Synthesis of the following inorganic compounds and their studies by IR, electronic spectra, Mossbauer and ESR spectra
- 3.1 $[Co(Py)_2Cl_2]$
- 3.2$[Ni(NH_3)_6]Cl_2$
- 3.3$[Cu(NH_3)_4]SO_4.H_2O$
- 3.4 Lanthanide complexes

4. Spectrophotometric Determination
- 4.1 Cu in a brass sample by spectrophotometer
- 4.2 Nitrate in water sample by colorimetric method
- 4.3 Ca and Mg in milk and egg.

5. Sodium and potassium by flame photometric method

Reference books:

1. Experimental Inorganic Chemistry by W.G. Palmer,Cambridge.
2. Inorganic Synthesis, MC GrawHill.
3. Handbook of Preparative Inorganic chemistry Vol. I and II, Academicpress.
4. Standard methods of chemical analysis by W.W. Scaff, TechnicalPress.
5. Vogel's Qualitative Inorganic Analysis (revised), OrientLongman.
6. Vogel's textbook of quantitative Inorganic Analysis (revised). J. Besset, R.C. Denny,G.H.Jeffery and J. Mendhan,ELBS.

M.Sc. CHEMISTRY
SEMESTER - II

MCH- 202 Paper No:VII	ELEMENTS OF MATERIALS CHEMISTRY-II	Theory (Marks)		Total Credits (Marks)
		U.E (60)	I.A (40)	03 (100)

Objective: To help students gain insight into the Imperfections in Crystal Systems which generates different Optical and Electronic Properties, Phase transformation in Materials, Deterioration of Materials by Corrosion and Commercial Polymers, Polymerization Techniques and Polymer Properties

Unit I: Imperfection in Crystal Lattice **12 L**

Types of Crystal Defects: Points Imperfections; Line Imperfection; Surface Imperfection; Creation of Vacancies: Interstitial and Substitutonal; 2D Imperfections: Edge and Screw dislocation, Twining stacking fault and low and high angle sub grain boundary, Motion of dislocation, Buerger's vector, effect of dislocation on mechanical properties of materials. Defect Clusters: Extended defects Split Interstitial, Koch Cluster; Crystallographic shear structure

Unit II: Phase Transformation and Elastic Deformation **08 L**

Time Scale for phase changes. Nucleation and Growth, Nucleation Kinetics; Homogeneous and Heterogeneous Nucleation; Growth and overall transformation Kinetics. Martensitic transformation, Buerger's classification: reconstructive and Displacive transformation Elastic Deformation, Modulus of Elasticity as a Parameter of Design; Resolved Shear stress, Relationship of slip and crystal structure of materials; Law of Critical Resolved Shear Stress

Unit III: **10 L**

Ziegler-Natta Co-ordination polymerization, Ring-Opening Polymerization of Ethers, Lactones and Lactams,Polymers of commercial importance: Polyethylene, Polypropylene, Polyvinyl Chloride, Polystyrene and Polturethanes, Mass Polymerization Techniques: Suspension and Emulsion Methods, Mechanical properties of polymers: stress-strain behaviour, tensile strength, elongation at break, Young's modulus and toughness of polymers

Unit IV Corrosion **14 L**

Classification of Corrosion: Chemical Corrosion; Electrochemical Corrosion; Forms of Corrosion: Uniform, Bimetallic, Crevice, Intergranular , Selective Leaching, Pitting, Stress, Erosion, Hydrogen Embrittlement, Cell Potential and EMF Series, Activation and Concentration Polarization ,Combined Polarization, Mixed Potential Theory, Mixed electrode, High Temperature Oxide Fromation, Thermodynamics of High Temperature Oxide, Pilling Bed Worth Ratio, Rate laws of Oxidation : Linear, Parabolic and Logarithmic

Essential Reading:

1. Corrosion Engineering by Mars and Fontana
2. Material Science and Engineering by Raghavan
3. Solid state Chemistry by A.R.West
4. Introduction to Polymers by R. J. Young and P. A.Lovell

M.Sc. CHEMISTRY
SEMESTER - II

Suggested Reading:

1. Introduction to Solid State Chemistry A.R.West
2. Materials Science and Engineering: An Introduction, W.D. Callister,Wiley
3. Text Book of Polymer Science by F. W.Billmeyer
4. Principles of Polymerization by G.Odian
5. Polymer Science and Technology of Plastics and Rubbers by P.Ghosh

M.Sc. CHEMISTRY
SEMESTER - II

Practical Course work

MCH-202L	ELEMENTS OF MATERIALS CHEMISTRY PRACTICAL -II	Practical (Marks)		Total Credits
		UE (25)	IA (25)	01 (50)

S. No	Experiment
1.	To prepare polymethyl methacrylate by bulk method and determine its % yield andsolubility.
2.	To prepare Phenol-Formaldehyde Resins (Resoles and Novolak).
3.	To study the kinetics of aqueous corrosion of mild steel by weight loss method the GMD.
4.	To prepare Al_2O_3 by Precipitation Method and Determine its Density.
5.	To Study the Phase Equilbria Diagram of Pb-Sn system by Direct Cooling Curve Method
6.	To determine the porosity and density of a given ceramic cube.
7.	To prepare a copolymer by bulk method and determine its % yield and solubility

Reference books:

1. Laboratory manuals prepared by Teacher-In-charge
2. A laboratory Manual of Metals and Alloys by S.M. Asharaf, Sharif Ahmad and Ufana Riaz
3. A laboratory Manual of Polymers by S.M. Asharaf, Sharif Ahmad and Ufana Riaz

M.Sc. CHEMISTRY
SEMESTER - II

MCH-203 Paper No:VIII	PERICYCLIC REACTIONS ANDPHOTOCHEMISTRY	Theory (Marks)		Total Credits (Marks)
		U.E (60)	I.A (40)	03 (100)

Objective: To help students gain insight about Pericyclic Reactions and Photochemistry

Unit I: Electrocyclic Reactions **12 L**

General pericyclic selection rules and their applications, Frontier molecular, orbitals of ethylene, 1,3-butadiene, 1,3,5-herxatriene, 1,3,5,7-octatectraene and allyl systems. Electrocyclic reactions: conrotatory and disrotatory motions of 4nπ, [4n+2]π, and allyl systems. Correlation diagrams for 4π-electrons and 6π-electrons systems, torque selectivity (a special kind of selectivity in pericyclic reactions), and pericyclic reactions of ionic species including Nazarov cyclization reaction.

Unit II Cycloaddition and Sigmatropic Reactions **08 L**

General orbital symmetry rules: [2+2] cycloaddition reactions, [2+2+2] cycloaddition reactions, [4+2] cycloaddition reactions, [6+4] cycloaddition reactions, [5+2] cycloaddition reactions, [8+2] cycloaddition reactions, [14+2] cycloaddition reactions, cheletropic cycloaddition and cycloreversion reactions, 1,3-dipolar cycloadditions including click chemistry; Sigmatropic reactions: (1,3), (1,5), (1,7), (2,3), (3,3), Ene reaction, Studinger reaction, and some other group transfer reactions. **10 L**

Unit III: Basics and Photochemistry of Aromatic Compounds

Excited states and ground state, singlet and triplet states. forbidden transitions, fate of the excited molecules: Jablonski diagram, fluorescence and phosphorescence, the determination of photochemical mechanism and quantum yield. Isomerizations, skeletal isomerizations, and singlet oxygen reactions. Photo Fries rearrangement of ethers and anilides. Synthetic applications of Barton and Hoffman-Loefller Freytag reactions. **14 L**

Unit IV Photochemistry of Alkenes and Carbonyl Compounds

Cis-trans isomerization, non-vertical energy transfer; photochemical additions; reactions of 1,3-, 1,4- and 1,5-dienes: Di-pie-methane rearrangement, Photochemistry of carbonyl compounds: Norrish type I & II reactions (cyclic and acyclic), α,β-unsaturated ketones; β,γ-unsaturated ketones; cyclohexenones (conjugated), Paterno–Buchi and de Mayo reactions, photooxidation and photoreduction.

Essential Reading

1. Advanced Organic Chemistry; Jerry March, Fourth edition, Wiley & Sons,(2007).
2. Carruthers, W. and Coldham, I. Modern methods of organic synthesis, Cambridge University Press(2004).
3. Fleming, I. Pericyclic reactions, Oxford science publication (1998)

Suggested Reading

1. Photochemistry and pericyclic reactions by jagdamba Singh and Jaya Singh, NewAcademic Science,2009.
2. Cox, A. and Camp, T. Introduction to Photochemistry,McGraw-Hill
3. Turro, N. J. and Benjamin, W. A. MolecularPhotochemistry

M.Sc. CHEMISTRY
SEMESTER - II

Practical Course work

MCH-203L	ORGANIC CHEMISTRY PRACTICAL -II	Practical (Marks)		Total Credits (Marks)
		IA (25)	UE (25)	01 (50)

S. No	Experiment
1.	Estimation of glucose, amino group, phenol, and amino acids.
2.	Small scale synthesis and purification of the following: 2.1 Succinic anhydride from succinic acid 2.2 Diethyl phthalate from phthalic anhydride 2.3 Acetophenone to oxime 2.4 Anthrone from Anthracene 2.5 Fries rearrangement: Phenylacetate 2.6 Mannich reaction 2.7 Cannizzaro reaction 2.8 Aldol condensation 2.9 Diazotization couplings 2.10 Phenolphthalein from phthalic anhydride.
3.	UV, IR spectra and melting points of simple compounds.

Reference books:

1. A.I. Vogel, Practical Organic Chemistry.
2. Comprehensive Practical Organic Chemistry by V. K. Ahluwalia.
3. Advanced practical (Organic Chemistry) by N. K. Vishnoi.

M.Sc. CHEMISTRY
SEMESTER - II

MCH-204 Paper: IX	Macromolecules & Surface Chemistry	Theory (Marks)		Total Credits (Marks)
		U.E. (60)	I.A. (40)	03 (100)

Objective: To help students gain insight about Surface chemistry and its Physical Characteristics

Unit I: Surface Phenomenon **08 L**

Surface tension, Capillary action, Surface films (Electro-kinetic phenomenon), Catalytic activity at surfaces. Catalysis on metal surfaces, Metal oxide surfaces. Application of photoelectron spectroscopy, ESCA and Auger spectroscopy to the study of surfaces.

Unit II: Interfacial Phenomenon **12 L**

Surface active agents, Classification of Surface-active agents, Co-surfactants, Micellization, Microemulsions, Aggregate structures of surfactants, Critical Micellar Concentration, Surfactant packing parameter, Kraft temperature, Factors affecting the CMC of surfactants, Counter ion binding to micelles, Hydrophobic interaction, Thermodynamics of micellization, Mass action models, Solubilization and Phase diagram of ternary microemulsion system.

Unit III: Macromolecules-I **15 L**

Classification and Chain configuration of macromolecules, Isotactic polymers, Atactic polymers, Syndiotactic polymers, Graft polymers, Electrically conducting polymers. Polymerization reactions, Kinetics of polymerization, Mechanism of polymerization.

Polymer microstructure: Microstructure based on chemical structure and geometrical structure. Meaning of glass transition temperature (*Tg*), factors influencing the glass transition temperature, importance of glass transition temperature and molecular weight.

Unit IV: Macromolecules-II **15 L**

Concepts of number average and mass average molecular weights. Methods of determining molecular weights (osmometry, viscometry, sedimentation equilibrium methods). Theta state of polymers. Distribution of chain lengths. 1-D random walk model in detail, Average end-to-end distance.

Properties of an isolated polymer molecule: Ideal chain, Freely-joined Gaussian chain, Distribution of segments in polymer chain, non-ideal chain, excluded volume, Dimension of real chains and scaling laws, Self-avoiding walk.

Concentrated solution and melts: Thermodynamic properties of polymer solutions, concentration fluctuation in polymer solutions, polymer blends, block copolymer.

Molecular motion of polymers in dilute solution: General theory of Brownian motion, Rouse and Zimm Bead spring models, hydrodynamics interactions, dynamic light scattering.

Essential Reading:

1. PHYSICAL CHEMISTRY 8TH ED., P. W. ATKINS AND J. DE PAULA, OXFORD UNIVERSITY PRESS, 2006.
2. PHYSICAL CHEMISTRY OF SURFACES - A. W. ADAMSON - JOHN WILEYSONS.
3. CATALYTIC CHEMISTRY, BRUCE C. GATES, JOHN WILEY & SONS, INC. 1992.(541.395GAT)
4. CATALYSIS AT SURFACES, I. M. CAMPBELL, CHAPMAN AND HALL, NEW YORK, 1998.
5. TERAOKA, I., POLYMER SOLUTIONS, WILEY-INTERSCIENCE, A JOHN WILEY & SONS INC. (2002).
6. DOI, M., THE INTRODUCTION OF POLYMER PHYSICS, CLARENDON PRESS OXFORD (1995).

7. DEGENNES, P. G. SCALING CONCEPTS IN POLYMER PHYSICS CORNELL UNIVERSITY PRESS (1979).
8. YOUNG, R. J. & LOVELL, P. A. INTRODUCTION TO POLYMERS 2ND ED. CHAPMAN & HALL (1991).

Suggested Reading:

1. PRINCIPALS OF NANOSCIENCE AND NANOTECHNOLOGY, M. A. SHAH AND TOKEER AHMAD, NAROSA PUBLICATIONS, 2010.
2. NANO SCIENCE & TECHNOLOGY, M. A. SHAH AND TOKEER AHMAD, I. K. INTERNATIONAL PVT LTD., 2021.
3. INTRODUCTION TO COLLOID AND SURFACE CHEMISTRY 2ND ED., D. J. SHAW, BUTTERWORTHS, 1970
4. MICELLES, THEORETICAL AND APPLIED ASPECTS, Y. MOROI, PLENUM PRESS, NEWYORK.
5. INTRODUCTION TO POLYMER SCIENCE, V. R. GOWARIKAR, N. V. VISHWANATHAN AND J. SRIDHAR-WILEYEASTERN

M.Sc. CHEMISTRY
SEMESTER - II

Practical Course work

MCH-204L	PHYSICAL CHEMISTRY PRACTICAL -II	Practical (Marks)		Total Credits
		I.A (25)	U.E (25)	01 (50)

S. No	Experiment
1.	Determine the cell constant of the given conductivity cell at room temperature.
2.	Determine the equivalent conductance at infinite dilution for acetic acid by applying Kohlrausch's Law of independent migration of ions.
3.	Determine the equivalent conductance, degree of dissociation and dissociation constant of acetic acid.
4.	Find out strength of weak and strong acids in a given mixture by conductometric titration.
5.	Find out solubility and solubility product of the given sparingly soluble salt in water.
6.	Find CMC of a given surfactant and, hence, calculate ΔG_{mix} of the surfactant.
7.	Verify Debye - Huckel equation for a strong electrolyte in water.
8.	Determine the electrode potentials of zinc and copper electrodes in 0.1 M and 0.01 M Solutions and calculate E_O values for these electrodes.
9.	Preparation of buffer solution of various pH and determine their pH values.
10.	Determination of solubility and solubility product by e.m.f method.
11.	Perform acid-base titration by pH metric method.
12.	Find out the first and second ionization constant of H_3PO_4 by pH metric method.
13.	Verify Beer Lambert Law. Determine the concentrations of $KMnO_4$ and K_2Cr_2O7 in a given unknown mixture.

Reference books:

1. Harris, D. C. Quantitative Chemical Analysis 6th Ed. W. H. Freeman & Co.(2002).
2. Experiments in Physical Chemistry, R.C. Das and B. Behra – Tata McGrawHill.
3. Advanced Practical Physical Chemistry, J.B. Yadav - Goel PublishingHouse.
4. Advanced Experimental Chemistry, Vol. I - Physical, J.N. Gurtu and R. Kapoor–S. Chand & Co.
5. Selected Experiments in Physical Chemistry, N.G. Mukherjee – J.N. Ghose &Sons.
6. Experiments in Physical Chemistry, J.C. Ghosh - Bharti Bhavan.
7. Senior Practical Physical Chemistry, B.D. Khosla; V.C. Garg, Adarsh Khosla R. Chand &Co

M.Sc. CHEMISTRY
SEMESTER - II

MCH-205 Paper: X	GROUP THEORY AND SPECTROSCOPY	Theory (Marks)		Total Credits (Marks)
		U.E(60)	I.A(40)	04 (100)

Objective: The unit deals with the advance concepts of Spectroscopic Techniques

Unit –I: Infrared spectroscopy **12 L**

Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strength; anharmonicity, Morse potential energy diagram, Derivation of selection rules for diatomic molecules based on harmonic oscillator approximation. Dissociation energies from vibrational data. Rotational spectroscopy of diatomic molecules based on rigid rotator approximation. Determination of bond lengths and/ or atomic masses from microwave data. Effect of isotopic substitution. Non-rigid rotator. Vibrational-rotation spectroscopy, P, Q and R branches. Breakdown of Born-Oppenheimer approximation

Unit-II: Raman Spectroscopy **12 L**

Classical and quantum theories of Raman effect. Stokes and anti-Stokes lines. Polarizability ellipsoids. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules. Selection rules, mutual exclusion principle. Polarization of Raman lines.
Resonance Raman spectroscopy, coherent anti Stokes Raman spectroscopy (CARS).

Unit III: Nuclear Magnetic Resonance **10 L**

Nuclear spin, resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors Influencing coupling constant 'J', spin decoupling; Basic ideas about instrument, NMR studies of nuclei other than proton – ^{13}C, ^{19}F and ^{31}P. FT-NMR, advantages of FT-NMR.

Unit IV: Paramagnetic Resonance Spectroscopy **15 L**

Electron Spectroscopy: Introduction-representation of the spectrum- hyperfine splitting in some simple system. Hyperfine, splitting in various structures (methyl radical and bis-(salicylaldimine)copper(II)). Factors affecting the magnitude of 'g' values. Zero field Splitting and Kramers degeneracy

Essential Reading:

1. Modern Spectroscopy, J.M. Hollas, John Wiley & Sons(2004).
2. NMR, NQR, EPR and Mössbauer Spectroscopy in Inorganic Chemistry, R. V. Parish, EllisHarwood.

Suggested Reading:

1. Basic Principles of Spectroscopy, R. Chang, McGraw Hill, N.Y. (1970).
2. Theory and Applications of UV Spectroscopy, H.H. Jaffe and M. Orchin, and IBH-Oxford.
3. Fundamentals of Molecular Spectroscopy, Fourth Edition, C.N. Banwell and E.M. McCash, TataMcGraw-Hill Publishing Company Limited, New Delhi(1994).
4. Molecular Spectra and Molecular Structure – I : Spectra of Diatomic Molecules, Gerhard Herzberg, D. Van Nostrand Company, Inc. Princeton, New Jersey, 1950 (539.12 HER51323)
5. Modern Molecular Spectroscopy, HS Randhawa, MacMillan India Ltd., 2003.

M.Sc. CHEMISTRY
SEMESTER - II

MCH-206 Paper: XI	Mathematical & Computational Methods in Chemistry	Theory(Marks)		Total Credits (Marks)
		U.E.(60)	I.A.(40)	04 (100)

Objective: The skill paper deals with fundamental knowledge of mathematical methods in chemistry and its implementation with C-programming. At the end of this course, the student should be able to choose and apply most relevant mathematical and computational models to solve a given experimental or theoretical chemistry problem.

Unit I:

Refreshing Basic Mathematics: Algebra, e.g. equations, matrices, determinants, number systems, series summations, etc., Geometry, Co-ordinate Geometry, e.g. straight lines, circles, conic section, etc., Calculus, e.g. functions, limits, derivatives etc., Taylor and McLaurin series expansion. **10 L**

Vectors: Vector Algebra; Properties of vectors under rotations. Scalar product and its invariance under rotations, Vector product, Scalar triple product and their interpretation in terms of area and volume respectively, Scalar and Vector fields. Vector Calculus; Differentiation and integration of vectors, scalar and vector fields, concept of gradient, divergence, curl, Jacobian and Laplacian in Cartesian, Sphericalpolar and Cylindrical Coordinate systems.

Operators & Matrices: Linear and Hermitian operators. Commutation of operators, Ladder operators and recursion relations of Hermite polynomials, Generating functions, Rodrigues's representation. Matrices as linear operators, geometrical operations. Special types of square matrices. Eigenvectors and eigenvalues of Hermitian and unitary matrices. Cayley-Hamilton theorem, degenerate eigenvalues. Gram-Schmidt orthogonalization. Diagonalization of matrices

Unit II:

Approximation: Taylor and binomial series (statements only), Ordinary differential equations (ODE) and Partial differential equations: Linear independence. General solution of homogeneous equations. Power series solutions. Ordinary and singular points of an ODE. First Order Differential Equations and Integrating Factor, Second Order Differential equations: Homogeneous Equations with constant coefficients, Wronskian and general solution, Statement of existence and Uniqueness Theorem for Initialn Value Problems, Particular Integral. **08 L**

Calculus of functions of more than one variable: Partial derivatives, exact and inexact differentials. Integrating factor, with simple illustration, Constrained Maximization using Lagrange Multipliers.

Unit III:

Fourier Transformation: Fourier series, sine, cosine and exponential Fourier series. Fourier transform, Fourier sine and cosine transforms, applications of Fourier transforms. **12 L**

Laplace Transformation: Laplace transform and its inverse, Solution of initial value problems using Laplace transform.

Special functions: Properties of Legendre polynomials. Rodrigues' formula, Generalized Fourier-Legendre series, generating function, Recursion formulae, Associated Legendre polynomials. Hermite, Laguerre and associated Laguerre polynomials.

M.Sc. CHEMISTRY
SEMESTER - II

Unit-IV:

Basics of C Programming: Elements of C Language. Types of C Constants, Variables, Instructions inbuilt functions. arithmetic expressions, hierarchy of operations, use of parenthesis, modulus operator. C keywords and commands. Control instructions; Arrays, declaring an array, initializing an array, break statement, strings and character arrays, sorting an array, finding maximum and minimum in an array, multidimensional arrays. File I/O (Input and Output). *Hands on training.* **12 L**

Numerical Methods: Solution of quadratic equation by formula, Numerical methods for the roots of polynomial equations, numerical differentiation, integration (Trapezoidal rule, Simpson's rule). Solution of ordinary differential equation, matrix inversion and diagonalization - the Jacobi transformation for the diagonalization of a symmetric matrix. *Application of Numerical methods to Chemistry.*

ESSENTIAL READING:

1. MATHEMATICAL METHODS FOR PHYSICISTS, G. B. ARFKEN, H. J. WEBER, F. E. HARRIS (2013,7TH ED, ELSEVIER)
2. ERWIN KREYSZIG, ADVANCED ENGINEERING MATHEMATICS, (WILEY INDIA)
3. R. G. MORTIMER, MATHEMATICS FOR PHYSICAL CHEMISTRY, 2ND ED. ELSEVIER (2005).
4. DONALD A. MCQUARRIE, MATHEMATICS FOR PHYSICAL CHEMISTRY: OPENING DOORS, (2008)
5. FREE C COMPILERS FOR WINDOWS ARE AVAILABLE AT:
(I) HTTP://WWW.CPROGRAMMING.COM/CODE_BLOCKS/, INSTRUCTIONS FOR SETTING UP C COMPILER IS GIVEN ON THIS URL.
(II) HTTP://DOWNLOAD.SAVANNAH.GNU.ORG/RELEASES/TINYCC/, YOU CAN DOWNLOAD EITHER TCC-0.9.27- WIN32-BIN.ZIP OR TCC-0.9.26-WIN64-BIN.ZIP.
6. C IN DEPTH, S.K. SRIVASTAVA AND DEEPALI SRIVASTAVA, BPB PUBLICATIONS, NEW DELHI, 3RD EDITION, 2017.
7. YASHAVANT P. KANETKAR, LET US C 5THED., BPB PUBLICATIONS (2004)
8. RAMAN, K.V., COMPUTERS IN CHEMISTRY, TATA MCGRAW HILL EDUCATION PRIVATE LIMITED, 2011.
9. JURS, PETER C., ISENHOUR, THOMAS L. AND WILKINS, CHARLES L. BASIC PROGRAMMING FOR CHEMISTS: AN INTRODUCTION, WILEY-BLACKWELL (1987).
10. BALAGURUSAMY, E. NUMERICAL METHODS, TATA MCGRAW HILL (2000).
11. V. RAJARAMAN, COMPUTER ORIENTATED NUMERICAL METHODS, PHI LEARNING PVT. LTD. (2018).

M.Sc. CHEMISTRY
SEMESTER - III

MCH-301 **Paper no: XII(i)**	**NMR SPECTROSCOPY AND LANTHANIDE SHIFT REAGENTS**	**Theory(Marks)**		**Total Credits (Marks)**
		U.E(60)	**I.A(40)**	**03 (100)**

Objective: Introduction to advance concepts in NMR and Lanthanide shift reagents

10L

Unit I: Lanthanide Complexes of β-Diketones: Introduction, Overview of β-diketone ligands and types of complexes. Synthesis, Structural, Physical and Chemical properties. Volatile *β*-diketone complexes.

Unit II: Applications of Nuclear Magnetic Resonance Spectroscopy **12L**

Applications of spin-spin coupling to structure determination.: $Rh(\phi_3P)_3CI_3$, Diphosphate anion (HP_2O_{53}-), SbF_5, Measurement of magnetic susceptibility by NMR., NMR of paramagnetic transition metal ion complexes- Contact and Pseudo contact shifts., Contact shift and Covalency, Contact shifts in coordinated pyridine.

14 L

Unit III: Lanthanide Shift Reagents
Historical development and general principles. NMR of paramagnetic lanthanide complexes –Nature of the shift. The lanthanide shift reagents. Relative shifting and broadening abilities of the lanthanides. Hinckley's shift reagent. Effect of increasing coordination number of the lanthanide on the NMR spectra of added substrate.

Unit IV: NMR of Lanthanide Complexes **12 L**
NMR of dia and paramagnetic lanthanide(III) complexes, Complexes containing N-donor ligands,(b) Complexes of O-donors,(c) Mixed-ligand complexes,(d) Complexes with varying coordinates,(e) Study of NMR spectra of eight and ten-coordinated paramagnetic lanthanide Complexes,(f) Shift reagents as structural probes.,(g) Effect of aromatic solvents on the spectra of lanthanide complexes.

Essential Reading

1. Physical Methods in Chemistry: by R.S.Drago.
2. NMR of Paramagnetic molecules-Principles and Applications, Edited by LaMar, Horrocksand Holm, Academic Press (N.Y.).

M.Sc. CHEMISTRY
SEMESTER - III

MCH-302 Paper No :XIII(i)	INORGANIC REACTION MECHANISM	Theory (Marks)		Total Credits (Marks)
		U.E. (60)	I.A. (40)	03 (100)

Objective: Introduction to advance concepts in Inorganic Reaction Mechanism

12 L

Unit I: Introduction to Inorganic Reaction Mechanism

Introduction to labile and inert octahedral complexes, interpretation of lability and inertness of transition metal complexes - Valence Bond and Crystal Field theories, factors affecting the lability of complex, transition state or activated complex, substrate, attacking reagents- electrophilic and nucleophilic, types of substitution reactions- nucleophilic or ligand substitution (SN) and electrophilic or Metal substitution (SE) reactions..

Unit II: Mechanism of Substitution Reactions in Octahedral Complexes **12 L**

Mechanism of nucleophilic substitution reactions in octahedral complexes SN_1 or dissociation and SN_2 or association (or displacement) mechanisms, hydrolysis reactions-mechanisms of acid Hydrolysis and base hydrolysis, reactions of octahedral Co(III) amine complexes.

14 L

Unit III: Mechanism of Substitution Reactions in Square Planar Complexes

Mechanism of substitution reactions in Pt(II) complexes, factors effecting the reactivity of square planar complexes, Trans-effect, theories of trans-effect-Grinberg's electrostatic polarization theory and Chatt and Orgel pi-bonding theory, application of trans-effect to synthesis of complexes.

Unit IV: Electron Transfer (or Oxidation -Reduction) Reaction **12 L**

Electron transfer reactions, mechanism of one-electron transfer reactions-outer sphere and inner sphere mechanisms, two-electron transfer reactions-complimentary and non-complimentary reactions, mechanism of two-electron transfer reactions.

Essential Reading

1. Inorganic Reaction Mechanism - F. Basolo & G. Pearson.
2. Inorganic Reaction Mechanism - J. O. Edwards
3. Langford, H. & Gray, H.B. *Ligand Substitution Processes* W.A. Benjamin

Suggested Reading:

1. Selected Topics in Inorganic Chemistry- Malik, Madan &Tuli.
2. Katakis, D. & Gordon, G. *Mechanism of Inorganic Reactions* John Wiley & Sons: N.Y.(1987).

M.Sc. CHEMISTRY
SEMESTER - III

MCH-303 Paper No :XIV(i)	ORGANOMETALLIC CHEMISTRY - I	Theory (Marks)		Total Credits (Marks)
		UE (60)	IA(40)	03 (100)

Objective: Introduction to fundamental concepts in organometallic chemistry

Unit I: Organometallics- Main Group and Transition Elements **12 L**

Introduction and classification of organometallic complexes. IUPAC nomenclature for metal-π-complexes, Ziese salt, bonding and structure- stability of metal-alkene complexes. Synthesis of organometallic complexes- direct synthesis, redistribution method, metal exchange, ligand exchange, addition reaction, cycIization, sigma-pi - rearrangements and substitution methods. Importance of organometallic complexes as reagents, additives and catalysts.

Unit II: Metal Carbonyls **12 L**

Structure, π-bonding, bonding modes of CO. Syntheses of metal carbonyls. Reactions of metal carbonyls. Carbonyl anions, cations and hydrides. Colman's reagents. Metal Nitrosyls

Unit III: Ligands; Alkenes, Alkynes, Alkyl and Aryl Groups with Higher Hapticity **14 L**

Models of alkene and alkyne – metal bonding. The concept of Umpolung. Pauson-Khand reaction. Cyclopentadienyl as ligand, Metal sandwich compounds, Ferrocene and its reactions. Schwartz's reagent and hydrozirconation. Arene π-complexes and their reactions. COT as ligand. Neutral spectator ligands.

Unit IV: Structure Elucidation and IR Spectroscopy of Organometallic Complexes **12 L**

Vibrational spectra and its applications. Study of complex compounds- factors controlling the character of vibrations of large molecules. Coordination of inorganic groups in metal π–complexes. Coordination of sulphate ions. Coordination of nitrate ions. Cyanate and thiocyanate complexes; study of bridged ligands. Coordination and Changes in the vibrations of C--O bonds. Coordination of alkenes and changes in vibration in C=C bonds.

Essential Reading

1. Metallo-organic Chemistry- Anthony J Pearson, John Wiley & Sons Inc,(1985)
2. Inorganic Chemistry – Principles of Structure & Reactivity, J E Huheey, Elllen A Keiter & Richard L Keiter, IV Edition(2005)
3. Introduction to metal pi-complex chemistry- M. Tsutsui, M.N. Levy, A. Nakamura,M.
4. Ichikawa and K. Mori, Plenum Press, New York I Heme(1970).
5. Organometallic ·Chemistry - R. C. Mehrotra & A. Singh, Wiley Eastern Ltd.(2000)

Suggested Reading:

1. Advanced Inorganic Chemistry - F. Albert Cotton, Geoffrey Wilkinson, Carlos A Murillo& Manfred Bochmann, VI Edition, John Wiley & Sons Inc(1999)
2. Principles and application of organotransition metal chemistry, J.P. Collman, L.S. Hegsdus, J.R. Norton andR.G. Finke, University Science Book.
3. The Organometallic Chemistry of the transition metals, R.H. Crabtree, John Wiley, (1988).

M.Sc. CHEMISTRY
SEMESTER - III

MCH-304 Paper No :XV(i)	BIO-INORGANIC CHEMISTRY–I	Theory (Marks)		Total Credits (Marks)
		U.E. (60)	I.A. (40)	03 (100)

Objective: Introduction to fundamental concepts in Bioinorganic Chemistry

12 L

Unit I: Metal Ions in Biological System

Occurrence and availability of Inorganic elements in organism, transport and storage of Inorganic elements, Dose response of an element, biological function of inorganic elements,beneficial and toxic elements, essential and trace metals.

Unit II: Metal Storage, Transport and Biomineralization **12 L**

Sidrophore, phytosidrophores, ferretin, fransferrin, hemosiderine, biomineralization, assembly of advanced materials e.g. calcium phosphate, calcium carbonate, iron biominerals.

14 L

Unit III: Uptake, Transport and Storage of Inorganic Molecule

Oxygen transport and storage through hemoglobin and myglobin, Alternative oxygen transport in lower organisms. Photosynthesis: Photochemistry, absorption spectra of photosynthetic pigments, photophosphorylation - energy conversion process.

Unit IV: Transport and Function of Alkali and Alkaline Earth Metals **12 L**

Roll of Alkali and alkaline earth metals in neuro sensation. Ion Channels, ion pumps, magnesium catalysis of phosphate, ubiquitous regulatory role of calcium.

Essential Reading

1. Principles of Bioinorganic Chemistry S.J. Lippard and J. M. Berg, University Science Books.
2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J. S. Valentine, UniversityScience Books.
3. Inorganic Biochemistry, Vols. I and II, Ed. G. L. Eichhorn, Elsevier.

Suggested Reading:

1. Progress in Inorganic Chemistry, Vols. 18 and 38, Ed. J.J. Lippard, Wiley.
2. Inorganic Chemistry, James E. Huheey, Harper International, Sixth Edition (1983).

M.Sc. CHEMISTRY
SEMESTER - III

Practical Course Work

INORGANIC CHEMISTRY PRACTICAL -III MCHIL	Theory(Marks)		Total Credits (Marks)
	U.E (60)	I.A (40)	04 (100)

S. No **EXPERIMENT**

1. **Synthesis of inorganic compounds**
   Preparation of following compounds and their study by IR, electronic spectra, Mossbauer, ESR and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds involving vacuum lines.
   1.1 Synthesis and thermal analysis of group 2 metal oxalate hydrate.
   1.2 Synthesis of metal acetylacetonate; magnetic, IR, NMR studies.
   1.3 Magnetic moment of $Cu(acac)_2.H_2O$.
   1.4 *Cis*- and *Trans*-$[Co(en)_2Cl_2]$

2. **Spectrophotometric Determination**
   2.1 Mn/Cr/V in steel sample
   2.2 Mo/W/V/U/ by extractive spectrophotometric method
   2.3 F^- / NO_2^- / PO_4^{3-}
   2.4 Iron-phenanthroline complex: Jobs method of continuous variations.
   2.5 Zr-Alizarin Red-S complex: Mole ratio method.
   2.6 Cu-Ethylenediamine complex: Slope-Ratio Method

3. **Chromatographic Separations**
   (a) Cd and Zn.

Reference Books:

1. Experimental Inorganic Chemistry by W.G. Palmer, Cambridge.
2. Inorganic Synthesis, MC Graw Hill.
3. Handbook of Preparative Inorganic chemistry Vol. I and II, Academic press.
4. Standard methods of Chemical analysis by W.W. Scaff, Technical Press.
5. Vogel's Qualitative Inorganic Analysis (revised), Orient Longman.
6. Vogel's textbook of quantitative Inorganic Analysis (revised).

M.Sc. CHEMISTRY
SEMESTER - III

MCH-305 Paper No :XII(ii)	CONVENTIONAL CERAMICS	Theory (Marks)		Total Credits (Marks)
		U.E(60)	I.A(40)	03 (100)

Objective: Introduction to basic types in Ceramics materials and their applications

Unit I: Functional Ceramics **8 L**

General concepts, oxide and non-oxide ceramics- functions and applications; microstructure of ceramics; grain boundaries in ceramics, significance and their types, fabrication of polycrystalline ceramics- general aspect, brief treatment of synthesis of powders, forming processes, hot pressing, hot isostatic pressing

Structural Ceramics and their Properties

oxide ceramics- classification and general characteristics, non-oxide ceramics classification and general characteristics, general aspects and characteristics of alumina, zircona, silicon nitride, silicon carbide

Unit II: Ceramic Insulators **12 L**

Introduction, general aspects of linear dielectrics; glass- different types of glasses and their characteristics, selection criteria for glass insulators, important glass compositions and their thermal mechanical and electrical characteristics and applications, glass used in treatment of radioactive waste, laser glass, colored glass used in photograph.

Unit III: Ceramic Capacitors **14 L**

Significance of capacitors, history of development, ferroelectricity and capacitors, Basic capacitor materials- porcelain and steatite, rutile, barium titanate, solid solutions, fine grained materials, additives, relaxor dielectrics; classification of ceramic capacitors,- thick film capacitors, single layer discrete capacitors, multilayer capacitors, Basic multi-layer fabrication methods- lamination, stacking, spray deposition, build up process, electrode alloys; Barrier layer capacitors- composition, fabrication, characteristic, applications; capacitor performance parameters

Unit IV: Aerogel **14 L**

Introduction, Production of Aerogels, silica aerogels, organic aerogels, drying, structural investigations- aerogel structure, thermal and infrared optical properties and mechanical properties, applications

Essential Reading:

1. Introduction to Fine ceramics by Noburu Ichinose (ed.) John Wiley and Sons., New York (1987)
2. Ceramic Materials for Electronics – R.C. Buchanan (ed.) Marcel Deller, New York(1991)
3. Chemical Processing of Ceramics by Burtrand I. Lee, Edward J. A. Pope (ed) Marcel Deller, New York

Suggested Reading:

1. Modern Ceramic Engineering, Properties, Processing and Use in design, By David W. Richerson, Marcel Deller, NewYork

M.Sc. CHEMISTRY
SEMESTER - III

MCH-306 Paper No : XIII(ii)	BASIC CONCEPTS OF CRYSTALLOGRAPHY & CRYSTAL STRUCTURES	Theory (Marks)		Total Credits (Marks)
		U.E.(60)	I.A. (40)	03 (100)

Objective: Introduction to Crystallography and Single Crystal Growth Methods

Unit I: Crystal Lattice and Unit Cell **10 L**

Unit cell and Crystal lattices, brief concept of molecular symmetry, concept of Symmetry in crystal systems, ,Herman Mauguin notation for symmetry elements in crystal systems, representation of screw axis and glide planes ,restriction of symmetry elements in crystals systems, representation of lattice planes and directions , Bravias lattices, concept of Miller indices and Weiss indices ,hexagonal crystal system, Determination of miller indices in hexagonal systems, planes of form in crystals, zone rule, possible combination of rotational symmetries, determination of d spacing in crystals

Unit II: Point Groups and Space Groups in Crystal Systems **10 L**

Point groups in crystals systems, Herman Mauguin notation of point groups in crystal systems, centrosymmetric and non centrosymmetric point groups, representation of point groups in crystallography, Concept of space groups, structural elucidation of the following space groups: P1, C2, C2/m, $P222_1$, $I4_1$, determination of atomic coordinates and special positions of space groups ,systematic absent reflections, space group and crystal structure of perovskite (ABO_3)

Unit III: Packing in Crystals Structures **14 L**

Cubic close packing, hexagonal close packing, packing of ions ,alloys and molecular structures atomic coordinates and nomenclature ,structural relationships ,polyhedral representation of crystal systems ,packing of structures in terms of the distribution of tetrahedral sites ,octahedral sites and packing ions .Structural elucidation and distribution of interstitial sites in hcp structures : AX type - wurtzite (ZnS), nickel arsenide (NiAs); AX_2 type -rutile (TiO_2) cadmium Iodide (CdI_2),Structural elucidation and distribution of interstitial sites in ccp structures : AX type - rock salt (NaCl), sphalerite (ZnS), AX_2 type - cadmium chloride ($CdCl_2$), antifluorite(Na_2O), fluorite(CaF_2), classification and structures of silicates andspinels

Unit IV: Preparation of Single Crystals **12 L**

Czochralski method, Bridgman and stock Barger method, zone melting, flux method, Verneuli method ,vapor phase transport ,hydrothermal methods, high pressure hydrothermal methods vapour phase transport comparison of the different methods, dry high pressure methods, preparation of nanophase single materials by hydrothermal, microwave- and microwave-solvothermal methods, concept of epitaxial growth factors effecting growth of single crystal structures

Essential Reading:

1. Solid state Chemistry by A.R. West (Wiley)
2. Introduction to crystallography by D.P Sands And W.A. Benjamin.

Suggested Reading

1. Understanding solids: The science of materials by Richard Tilley (Wiley).

M.Sc. CHEMISTRY
SEMESTER - III

MCH-307 Paper No: XIV(ii)	POLYMER CHEMISTRY AND TECHNOLOGY	Theory (Marks)		Total Credits (Marks)
		UE (60)	IA (40)	03 (100)

Objective: Introduction to Polymer Physics and Characterization

Unit I: Polymer Physics **10 L**

Polymer Molecules, Conformation and Molecular Dimensions of Polymer Molecules, Properties of Isolated Polymer Molecules, Elasticity and Swelling of Polymer Gels, Molecular Motion of Polymers in Dilute Solutions, Amorphous Polymers, Structure of Amorphous Phase in Bulk Polymers, Mobility in Polymers, Glass Transition- Measurement of T_g, Effect of Various Parameters on T_g, Theoretical Interpretations, Crystallinity in Polymers, Determination of Degree of Crystallinity, Two Phase Structure of Semi-Crystalline Polymers and its Characterization and Correlation with Properties, Crystal Morphologies: Extended Chain Crystals, Chain Folding, Lamellae, Spherulite, Melting: Determination of Polymer Melting Point, The Effect of Various Parameters on Melting, Mechanical Properties: Stress-Strain Properties, Yield Behavior, Breaking Phenomena

Unit II: Polymer Characterization **10 L**

Thermodynamics of Polymer Solutions, Flory-Huggins and Lattice Theory of Polymer Solution, Entropy and Enthalpy of Mixing, Theta Temperature, Molecular Weight and Molecular Dimensions by Osmometry, Light Scattering, Viscometry and Gel Permeation Chromatography, Thermal Analysis of Polymers: Differential Scanning Calorimetry (DSC), Thermogravimetric Analysis (TGA) and Differential Thermal Analysis (DTA), Polymer Degradation and Stabilization

Unit III: Polymer Rheology **14 L**

Definition of Rheology, Geometry of Deformation, Newtonian and Non-Newtonian Behaviors, Measurement of Rheological Properties, Power Law, Free Volume Theory of Polymer Fluidity, Dynamic Flow Behavior, Time-Dependent Fluid Responses, Viscoelastic Properties, Mechanical Models of a Viscoelastic Material, Stress Relaxation, Creep and Relaxation behavior of Plastics

Unit IV: Polymer Technology **12 L**

Polymers of Commercial Importance, Mass Polymerization: Solution, Emulsion and Suspension Polymerizations, Ziegler Natta Coordination Polymerization, Metathesis Polymerization

Essential Reading:

1. Text Book of Polymer Science By F. W. Billmeyer
2. Introduction to Polymers by R. J. Young and P. A. Lovell
3. Polymer Chemistry by G. Challa

Suggested Reading

1. Polymers: Chemistry and Physics of Modern Materials by JMG Cowie
2. Principles of Polymerization by GeorgeOdian

M.Sc. CHEMISTRY
SEMESTER - III

MCH-308 Paper No: XV(ii)	CHEMISTRY OF ADVANCED MATERIALS	Theory(Marks)		Total Credits (Marks)
		U.E(60)	I.A(40)	03 (100)

Objective: Introduction to types of Advance materials and their applications

Unit I: Composite Materials **10 L**

Definition, General characteristics and classification, Matrix, Fillers, Types of matrix and fillers, Division of composites based on filler reinforcement pattern, Dispersion strengthened composites, Al-based (SAP) and Ni-based fibrous composites, Critical length of fibers, Effect of reinforcement pattern of fillers on mechanical properties of fibrous composites, types of fillers, Non-metallic and metallic composites:- Epoxy, Phenol, formaldehyde, Polyurethane based composites, Al, Mg, Ti, Ni- based fibrous composites, Applications of Composites

Unit II: Organic Conductors, Magnets & Super Conductors **10 L**

Introduction: Electrically conducting organic solids, Conjugate system: Polyacetylene, Polyaniline, Polypyrole, Polythiophene etc. Historical background general(Electron transfer salt based conductors, superconductors and Magnets) One dimensional conductors: Salts of partially oxidized Tetra cyano complexes, Quasi one and two dimensional conductors (TMTSF, BEDT-TTF, salts) tree dimensional conductors and superconductors fullerides and alkali metal doped fullerides. Para and Ferromagnetic conductors and superconductors

Unit III: Mesomorphic Materials (Liquid Crystal) **14 L**

Mesomorphic behaviour, thermotropic liquid crystal, positional rdr, bond orientational order, nematic and smectic mesophases, mectic-nematic transition and clearing temperature, homotropic, planer and schlieren textures, twisted nematics, chiral nematics, molecular arrangement in smectic. A and C smectic phases, optical properties of liquid crystals, dielectric susceptibility and dielectric constant. Optical storage memory switches and sensors

Unit IV: High Tc Materials **12 L**

Defect pervoskites, 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, Superconductivity state, heat capacity, coherence length, elastic constants, position life times, microwave absorption pairing and multigap structure in high Tc materials, application of high Tc materials

Essential Reading:

1. Principle of solid state, H. V. Keer, Wiley Eastern.
2. Handbook of Liquid Crystals, Kelkar and Hatz
3. Thermotropic Liquid Crystals, Ed., G. W. Groy, Chemie Verlog, John Wiley.

Suggested Reading

1. Materials Science by Azimasov (MirPublications)
2. Chemistry of Advanced Materials by Leonard V. Interrante and M.J. Hampden-Smith

M.Sc. CHEMISTRY
SEMESTER - III

ELEMENTS OF MATERIALS CHEMISTRY PRACTICAL-1 MCHML	**Practical (Marks)**		**Total Credits (Marks)**
	UE (60)	**IA (40)**	**04 (100)**

Practical Course Work

S. No	**EXPERIMENT**
1.	Prepare PMMA by suspension polymerization method and determine its molecular weight by viscometry.
2.	Prepare polystyrene by emulsion polymerization method and determine its viscosity average molecular weight.
3.	Prepare polyvinyl acetate by solution polymerization and synthesize polyvinyl alcohol from the prepared polymer by hydrolysis
4.	Prepare a copolymer of styrene and methylmethacrylate by solution method.
5.	Grow single crystals from the aqueous solutions of: (a) potash alum and (b) Rochelle salt.
6.	Determine the bulk density, porosity and specific gravity of the sintered clay piece
7.	Determine the band gap energy of Ge and Si crystals
8.	Study the kinetics of high temperature oxidation of mild steel.
9.	Synthesize cobalt ferrite ($CoFe_2O_4$) inverse spinel by chemical route.
10.	Measure the dielectric constant of Barium titanate, $BaTiO_3$.

Reference books:

2. Laboratory manual prepared by the Teacher–in-Charge
3. Crystal and crystal growing by Alam Holden and Phylis Singer
4. A laboratory manual of Polymers by S.M. Ashraf, Sharif Ahmad and Ufana Ria
5. Practical course in Polymer Chemistry by Pinner
6. Experiments in Polymer Chemistry by Billmeyer

M.Sc. CHEMISTRY
SEMESTER - III

MCH-309 Paper No :XII(iii)	METHODS IN ORGANIC SYNTHESIS	Theory (Marks)		Total Credits (Marks)
		UE(60)	IA(40)	03 (100)

Objective: The unit comprises of methods adopted for Organic Synthesis

Unit I Formation of C-C single bonds

Generation of thermodynamic and kinetic enolates Alkylation of enolates and enamines, Silyl enol ethers, Conjugate addition reactions of enolates and enamines, Michael addition, Aldol reactions, Evansaldol reaction, Mukaiyama aldol reaction and stereoselective aldol reactions. Baylis-Hillman, Robinson annulation, and Prins cyclization reaction. **8 L**

Unit II: Formation of C-C double bonds

Phosphorous ylides (Wittig, Horner-Wadsworth-Emmons and Arbuzov reactions), Preparation and application of sulphur ylides (Comparison of action and reactivity of phosphorous and sulphur ylides, Corey-Chaykovsky reaction. Preparation and uses of 1,3-dithiane in organic synthesis (umpolung or reversal of polarity), role of silicon in organic synthesis, origin and consequence of alpha effect and beta effect involving silicon compounds, Formation of alkenes: Shapiro, Bamford-Stevens, Julia, Peterson, Petasis, Corey-Winter, McMurry and Ramberg-Backlund olefinations. Alkenes formation using titanium and chromium reagents. **12 L**

Unit III: Oxidations

Oxidation of hydrocarbons (alkanes, alkenes, and aromatic hydrocarbons): Selenium dioxide, DDQ, Etard's and related reaction, epoxidation, Sharpless asymmetric epoxidation, kinetic resolution of chiral allylic alcohol, Prevost and Woodward dihydroxilation, Sharpless asymmetric dihydroxilation. Asymmetric amino-hydroxilation. Palladium catalyzed oxidation of alkenes. Oxidation of alcohols: Chromium reagents, oxidation via alkoxysulfonium salts (DCC &. Swern oxidation), manganese reagents (MnO_2, PCC, Jones reagent, Collins reagent) other metal based oxidants (Ag_2CO_3, RuO_4 and $Tl(NO_3)_3$) oxidative cleavage of C-C bonds. Oxidation of alpha, beta-unsaturated ketones. **08 L**

Unit IV: Reductions

Catalytic hydrogenation: Of alkenes, alkynes, aromatic compounds, nitrile, oximes and nitro compounds. Heterogeneous and homogeneous catalysis, stereochemistry and mechanism. Induced asymmetry via homogeneous hydrogenation. Reduction by desolving metals: Of carbonyl compounds, aromatic compounds (Birch reduction), Alkynes and conjugated dienes. Hydride transfer reagents: Aluminium alkoxides (Meerwein-Pondorff-Verly reduction), Lithium aluminium hydride, sodium borohydride, sodium cyano borohydride and Diisobutyl aluminium hydride (DIBAL-H) Wolff-Kishner's reduction, reductionswith diimides and trialkyl tin hydrides. Enzymetic reductions**.** **14 L**

M.Sc. CHEMISTRY
SEMESTER - III

Essential Reading

1. Smith M. B & March, J. Advanced organic chemistry sixth edition, John Wiley & Sons (2007).
2. Carey, F. A. & Sundberg, R. J. Advanced Organic Chemistry, Parts A & B, Plenum: U.S.(2004).
3. Carruthers, W. and Coldham, I. Modern methods of organic synthesis, Cambridge UniversityPress (2004).

Suggested Reading

1. G. S. Zweifel and M. H. Nantz, Modern Organic Synthesis- An Introduction, W. H. Freeman and Company, 2006.
2. Bruckner, R. Advanced Organic Chemistry Elsevier(2002)
3. Clayden, Greeves, Warren & W others. Organic chemistry Oxford University press(2001)
4. Lowry, T. H. & Richardson, K. S. Mechanism and Theory in Organic Chemistry Addison-Wesley Educational Publishers, Inc.(1981).

M.Sc. CHEMISTRY
SEMESTER - III

MCH-310 Paper No: XIII(iii)	ADVANCED TOOLS IN ORGANIC SYNTHESIS	Theory(Marks)		Total Credits (Marks)
		UE(60)	IA(40)	03 (100)

Objective: The unit will help students to understand the various tools used in AdvanceOrganic Synthesis

Unit I Strategic applications of named reactions:

Mitsunobu, Appel, Nef, Henry, Pfitzinger, Bucherer, Kakis-kikuchi, Thiele, Thorpe, Skraup, Ritter, Kulinkovich, Tischenko, Stetter, Duff, Dakin, Chugaev, Regitz, Reissert, Deobner, Simmons-Smith, Sakurai, Corey- Fuchs, Corey-Bakshi-Shibata, Corey–Seebach, Chan alkyne, Nayori, Buchner, Pictet-Spengler, Takai, Rubottom, Reformatsky, Darzens, Stobbe, Staudinger, Barton-deoxygenation and decarboxylation, Ciamician–Dennsted, Vilsmeier–Haack, Weiss–Cook, Blanc, Allan–Robinson, Bergman, Parham cyclization, Weinreb amide, and Fischer indolization reactions. **12 L**

Unit II: Rearrangements

General mechanistic considerations-nature of migration, migratory aptitude, memoryeffects. Cationotropic and Anionotropic rearrangements. Rearrangements involving electron deficient Carbon, Nitrogen and Oxygen. A detailed study of the following rearrangements Pinacol-Pinacolone, Wagner Meerwein, Demjanov, Dienone- Phenol, Benzil-Benzilic acid, Favorskii, Arndt- Eistert, Neber, Rupe, Hoffmann, Losson, Curtius, Pummerer, Payne, Schmidt, Beckmann, Wittig, Wolff, Smile's, Mislow–Evans, Carroll, Overman, Meisenheimer and Baeyer-Villiger rearrangements. **12 L**

Unit III: Fragmentations

Basic concepts of fragmentations: Grob, Eschenmoser-Tanabe, Marshall, Warton, and some other important fragmentations. Basics of macro lactonization, modes of activations, applications of named reactions for macro-lactonization: Corey-Nicoloau, Venkataraman, Boden-Keck, Masamune, Shiina, Yamaguchi, Yamamoto, Mukaiyamaand Mitsnobu etc. **08 L**

Unit IV: Organometallics in organic synthesis

Basics, Hapticity, 18-electrons and Wade rules, metal clusters, sandwiched compounds, fluxional molecules, catalysis, Structure and bonding in metalalkyls, aryls, allyls, cyclopentadienyl and arene complexes, Oxidative-Addition and Insertion reactions at M-C bond & M-H bond, transmetallation and cyclization reaction, hydroformylation using cobalt octacarbonyl, Monsanto acetic acid process, Hydrogenation by Willkinsons catalyst, Tebbe reagent, Ziese's salt, metathesis, Wacker process, Pauson-Khand, Nicholas, Buchwald-Hartwig, Ziegler-Natta, Schwartz, coupling reactions: Heck, Suzuki, Stille, Sonogashira, Hiyama, Fukuyama, Negishi, Kumada, Chan-Lam, Castro- Stephan, Petasis, Glaser, Hay and Nozaki- Hiyama-Kishi, Tsuji-Trost allylation. **14L**

M.Sc. CHEMISTRY
SEMESTER - III

Essential Reading:

1. Kurti, L. and Czako, B. Strategic applications of Named reactions, in organic synthesis (2004).
2. Carruthers, W. and Coldham, I. Modern methods of organic synthesis, Cambridge University Press (2004).
3. G. S. Zweifel and M. H. Nantz, Modern Organic Synthesis- An Introduction, W. H. Freeman andCompany,2006

Suggested Reading:

1. Organometallic and bioinorganic chemistry by Ajay Kumar.
2. Organometallic Chemistry- R.C. Mehrotra & A. Singh, Wiley Eastern Ltd. (2000).

M.Sc. CHEMISTRY
SEMESTER - III

MCH-311 Paper No: XIV(iii)	REAGENTS AND ORGANIC SYNTHESIS	Theory (Marks)		Total Credits (Marks)
		U.E. (60)	I.A. (40)	03 (100)

Objective: The unit will help students to understand the various Reagents and the mechanism adopted in Organic Synthesis

Unit I Asymmetric Synthesis: **12 L**

Concise introduction to asymmetric synthesis, detailed discussion on resolution, chiral auxiliaries, chiral ligands, chiral catalysts and organo-catalysts with specific examples including newer methods involving enzymatic and catalytic reactions, enantio and diastereoselective synthesis. Introduction to domino/tandem/cascade reaction concepts with selected examples**..**

Unit II: Protecting of the following groups: Role of protective groups in organic synthesis, Protection of carbon-carbon double bonds, alcohols (including 1,2 and 1,3-diols), amine, thiol, carbonyl carboxyl groups, phenols and catechols **12 L**

Unit III: Disconnection approach to synthesis of organic molecules: **08 L**

An introduction to synthons and synthetic equivalents, conversion and interconversion of functional groups, selective reactions (chemo-, region-, and stereoselective), formation of C- C, C-O, C-N bonds.

Unit IV: Disconnection approach: **14L**

Alcohols and carbonyl compounds, consideration of regioselectivity. Alkene synthesis and uses of acetylenes in organic synthesis. (b) Two Group C-C Disconnection: Diels Alder reaction, 1,3-difunctionalised compounds, α,β-unsaturated carbonyl compounds, 1,5- difunctionalised compounds. Michael addition and Robinson Annulation. Functional group transformations.

Essential Reading:

1. L. F. Fieser and M. Fieser, Reagents for Organic Synthesis, Vol. 1-16 (Vol. 1, 1967), Wiley Interscience, NewYork.
2. M. B. Smith and J. March, March's Advanced Organic Chemistry – Reactions, Mechanisms & Structure, 5th ed. (2001), Wiley-Interscience, New York.
3. M. B. Smith, Organic Synthesis, McGraw Hill Inc., New York (1995).
4. J. Clayden, N. Greeves, S. Warren, and E. Wothers, Organic Chemistry, Oxford Univ. Press, Oxford(2001).

Suggested Reading:

1. P. R. Jenkins, Organometallic Reagents in Synthesis, Oxford science Publ., Oxford (1992).
2. Organometallics in organic synthesis – J. M. Swan and D. C. Black (Chapman and Hall).
3. Protective groups in Organic Synthesis Theodora W. Greene & Peter G.M. Wuts.

M.Sc. CHEMISTRY
SEMESTER - III

MCH-312 Paper No :XV(iii)	CHEMISTRY OF HETEROCYCLIC COMPOUNDS	Theory(Marks)		Total Credits (Marks)
		U.E(60)	I.A(40)	03 (100)

Objective: The unit will help students to understand the various types of Heterocyclic compounds

Unit I: Three and four membered heterocycles
Nomenclature of heterocyclic compounds, reactivity order of various three, membered and four membered heterocycles, Structure, synthesis and reactions, of aziridines, oxiranes, **12 L**

Unit II: Five and six membered heterocycles
Structure, preparation, properties and reactions of indole, quinoline and isoquinoline. Order of basicity and aromaticity of different heterocycles containing two hetero atoms. **12 L**

Unit III: Metallo-porphyrins
Basics, Heme and nonheme protein, oxygen uptake, structure and function of haemoglobin, myoglobin, hemocyanin, plastocyanin, hemoerytherine, cyanocobalamine, chlorophylls, and Iron-Sulfur proteins. **08 L**

Unit IV: Metallo-enzymes
Basics, chymotrypsin, carboxypeptidase, carbonic anhydrase, alcohol, dehydrogenase and aldehyde oxidase. Nitrogenase enzyme and role of Alkali, and Alkaline earth metal ions (Na^+, K^+, Ca^{2+}& Mg^{2+}) in Biological systems**.** **14 L**

Essential Reading:

1. T.L. Gilchrist, Heterocyclic Chemistry, 3rd Edition (1997) Addison-Wesley Longman Ltd.,England
2. A.R. Katritzky, C.A. Ramsden, J.A. Joule and V.V. Zhdankin, Handbook of Heterocyclic Chemistry, 3rd Edition (2010), Elsevier, Oxford, UK.
3. Heterocyclic Chemistry, 4th ed. J.A. joule and K. Mills Blackwell Publishing, Indian Reprint 2004.
4. Heterocyclic Chemistry Vol-III, 1st ed. R. R. Gupta, M. Kumar, V. Gupta
5. Springer-Verlag, Berlin Heidelberg Publication(2005)
6. Aromatic Heterocyclic Chemistry: David T. Davies, 1992, Oxford University
7. Bioinorganic Chemistry- A Short Course; R. M. Roat- Malone; Wiley Interscience; 2003.
8. Organometallics and bioinorganic chemistry by Ajay Kumar.

M.Sc. CHEMISTRY
SEMESTER - III

Suggested Reading:

1. Inorganic chemistry by D.F Shriver and P.W. Atkins.).
2. R.K. Bansal, Heterocyclic Chemistry: Syntheses, Reactions and Mechanisms,
3. 3rd Edition (1999), New Age International, Publisher, New Delhi.
4. P. R. Jenkins, Organometallic Reagents in Synthesis, Oxford science Publ., Oxford (1992).
5. Organometallics in organic synthesis – J. M. Swan and D. C. Black(Chapman and Hall).
6. Protective groups in Organic Synthesis Theodora W. Greene & Peter G.M. Wuts.

M.Sc. CHEMISTRY
SEMESTER - III

Practical Couse Work

ORGANIC CHEMISTRY PRACTICAL-I MCHOL	Practical (Marks)		Total Credits (Marks)
	UE (60)	IA (40)	04 (100)

S. No **EXPERIMENT**

1. Use of chemistry software like Chem draw, Chem office etc.
2. (a) Isolation of caffeine from tealeaves
   (b) Isolation of piperine from black pepper
   (c) Isolation of lycopene from tomatoes.
3. Preparations, isolation and characterizations: (one/two/three-stage).
   - 3.1 Diels-Alder reaction of anthracene with maleic anhydride
   - 3.2 Deils-alder reaction between furan and maleic acid
   - 3.3 Synthesis of indole from cylohexanone and phenylhydrazine.
   - 3.4 Para- aminoazobenzene fromaniline
   - 3.5 Benzophenone → Benzophenone oxime→ Benzanilide (Beckmann rearrangement)
   - 3.6 Anthrone from phthalic anhydride
   - 3.7 Benzoin → Benzil → Benzilic Acid.
   - 3.8 Nitrobenzene →m-dinitrobenzene → m-nitroaniline →m-nitrophenol.
   - 3.9 Phthalic anhydride → phthalimide → anthranilic acid.
   - 3.10 Eosin from phthalic anhydride
   - 3.11 Glucazone fromglucose
   - 3.12 Methylene blue from dimethylaniline

Reference Books

1. Vogel Practical Organic Chemistry.
2. Comprehensive Practical Organic Chemistry by V.K. Ahluwalia.
3. Advanced practical (organic chemistry) by N. K. Vishnoi.

M.Sc. CHEMISTRY
SEMESTER - III

MCH-313 Paper No :XII(iv)	ADVANCED STATISTICAL MECHANICS	Theory (Marks)		Total Credits (Marks)
		U.E(60)	I.A(40)	03 (100)

Objective: This paper will provide an advanced level in-depth understanding about various statistical theories of solids, liquids and imperfect gases and their applications. This course also introduces some basic concepts of computer simulations.

Unit-1: Ensembles

Grand Canonical Ensemble: Distribution functions in monatomic, one-component systems, Kirkwood-Salsburg integral equation Canonical Ensemble: Definition of distribution and correlation functions, Thermodynamic functions of a fluid and the radial distribution function, Potential of mean force and the superposition. approximation, Kirkwood integral equation, Bom-Green-Yvon (BGY) integral equation. HNC equation, PY equation, Fluid of hard spheres according to the superposition approximation, Fluid with modified Lennard-Jones molecular interaction potential according to the superposition approximation. **10L**

Unit-2: Theory of Imperfect Gases.

Partition functions and cluster integrals, Pressure of gas expressed as a power series in activity. Irreducible cluster integrals, Virial expansion for a gas, Calculation of Virial coefficients of an imperfect gas. Theory of condensation. **08L**

Unit-3: Lattice Statistics

Ising Model. Nearest neighbor lattice statistics-Thermodynamics and interconnections, Exact and formal methods. Computer simulation: Motivation and applications, Intermolecular potentials Molecular Dynamics and Monte Carlo Methods **12L**

Unit-4: Statistical Theory of Liquids-Supercooled and Ionic Liquids

Theories of transport properties; non-Arrhenius behaviour of transport properties, Cohen-Turnbull free volume model, configurational entropy model, Experimental Methods for Structure Determination: Spectroscopic techniques for liquid structure studies, Neutron and X-ray scattering. **12L**

RECOMMENDED TEXTS:

1. ALLEN, M. P. & TILDESLEY, D. J. COMPUTER SIMULATIONS OF LIQUIDS OXFORD SCIENCE PUBLICATIONS: OXFORD (1987).
2. HILL, T. L. STATISTICAL MECHANICS: PRINCIPLES AND SELECTED APPLICATIONS DOVER PUBLICATIONS INC.: NEW YORK (1987).
3. LANDAU, L. D. & LIPSHITZ, E. M. STATISTICAL PHYSICS VOL. 5, PART 1, 3RD ED., PERGAMON PRESS (1980).
4. MCQUARRIE, D. A. STATISTICAL MECHANICS VIVA BOOKS PVT. LTD.: NEW DELHI (2003).
5. BAGCHI B. STATISTICAL MECHANICS FOR CHEMISTRY AND MATERIAL SCIENCE, CRC PRESS (2018).

M.Sc. CHEMISTRY
SEMESTER - III

MCH-314 Paper No:XIII(iv)	ADVANCE SOLID STATECHEMISTRY	Theory (Marks)		Total Credits (Marks)
		U.E(60)	I.A(40)	03 (100)

Objective: The paper deals with the Advanced Concepts of Solid State Chemistry

Unit I Concepts of Solids

Crystalline and Amorphous Solid, Unit cell, Summary of crystal lattices, Reciprocal lattice, Bonding & packing in crystals, Lattice planes, Symmetry elements, Space lattice, Glide planes, Screw Axis, Point groups and notations of 32, 222, mm2 and mmm point groups, space groups and elucidations of representing point groups; viz. Monoclinic C2, Monoclinic C2/m, Orthorhombic $p222_1$ and Tetragonal $I4_1$. **11L**

Unit II: Crystal Defects and Non-Stoichiometry in Solids

Perfect and imperfect crystals, Intrinsic and extrinsic defects- point defects, line defects and plane defects, Schottky and Frenkel defects, Thermodynamics of Schottky and Frenkel defect formation, F, V & H Colour Centers, Non-stoichiometry in solids and their mathematical calculations. **10 L**

Unit III: Functional Properties of Solids

(a) Electrical Properties: Dielectric materials, Dielectric properties (dielectric constant and dielectric loss), Dependence of dielectric properties on size, Polarizability, Concepts of ferroelectricity, Pyroelectricity and Piezoelectricity. **15 L**

(b) Magnetic Properties: Classification of materials, Line of forces, Effect of temperature, Magnetic moment calculations, Ferro- and antiferromagnetic ordering, Dependence of magnetic properties on size, Magnetic domains and Hysteresis.

(c) Electronic Properties: Metals, Insulators, Semiconductors and Superconductors, Density of states, Origin of bands, E-k diagrams, Bonding in solids, Band theory, Intrinsic and extrinsic semiconductors p-n junction.

Unit IV: Structures of Solids

Perovskite structure (e.g. $CaTiO_3$ and $BaTiO_3$), Spinel structure (e.g. $MgAl_2O_4$), Rutile TiO_2 structure, Rock salt NaCl structure, Sphalerite and Wurtzite structures of ZnS, Ruddlesden-Popper type K_2NiF_4 (e.g. Sr_2TiO_4) and β-K_2SO_4 (e.g. Ba_2TiO_4) structures **08 L**

Essential Reading

1. Solid State Chemistry and its applications, Anthony R. West, John Wiley &Sons.
2. Solid State Chemistry, Lesley Smart and Elaine Moore, Chapman &Hall.
3. Solid State Chemistry Techniques, A. K. Cheetham and Peter Day, Oxford Science

Suggested Reading

1. New Directions in Solid State Chemistry, C. N. R. Rao and J. Gopalakrishnan, CambridgeUniversity Press.
2. Principals of Nanoscience and Nanotechnology, M. A. Shah and Tokeer Ahmad, NarosaPublications, 2010.
3. Principles of the Solid State, H. V. Keer, New Age International Publishers.
4. Solid State Chemistry, D. K. Chakrabarty, New Age International Publishers

M.Sc. CHEMISTRY
SEMESTER - III

MCH-315 Paper No :XIV(iv)	CHEMICAL KINETICS	Theory (Marks)		Total Credits (Marks)
		U.E(60)	I.A(40)	03 (100)

Objective: The unit deals with the advanced Concepts of reaction dynamics and chemical kinetics

Unit I: Statistical Theories of Kinetics **14 L**

Postulates and derivation of transition state theory, Potential energy surfaces, Thermodynamic formulations of transition state theory, Applications of transition state theory, Intermolecular energy transfer, Unimolecular reaction rate theory (Lindemann–Hinshelwood treatment), Rice- Ramsperger and Kassel (RRK) theory and Marcus's refinement of RRK theory (RRKM).

Unit II: Reaction Dynamics **12 L**

Introduction, Collision, Collision diameter, Collision theory, Collision cross section, Opacity function, Harpoon Mechanism, Experimental approaches i.e., Molecular beam scattering and state resolved spectroscopic techniques, Stripping and rebound mechanism, State to state kinetics.

Unit III: Complex Reactions **12 L**

Chain reactions, Oscillatory reactions, Photochemical reactions. Enzyme kinetics: Michaelis-Menten mechanism- single and double intermediates. King- Altman method for working out the kinetics of complex enzyme reactions. Enzyme catalysed reactions (various types of inhibition).

Unit IV: Kinetic Measurements **12 L**

Introduction, Initiation methods, Kinetic systems (i.e., Static systems, flow systems, and shock tubes), Description of techniques (i.e., Flash photolysis and laser flash photolysis, Absorption spectroscopy, Laser photolysis/Chemiluminescence, Laser-Induced fluorescence, and Photoionization techniques), Treatment of Kinetic data.

Essential Reading

1. Chemical kinetics by K.J. Laidler, Third Edition,1987.
2. Chemical Kinetics by L. Wilkinson.
3. Pilling, M.J. & Seakins, P.W., Reaction Kinetics, Oxford University Press (1995).
4. Chemical Kinetics and Dynamics by Jeffrey I. Steinfield, Joseph S. Francisco, William L. Hase, IInd Edition, 1998.

Suggested Reading

1. Chemical kinetics and Reaction Mechanism by James H. Espenson, 2nd Ed., McGraw-Hill,1995
2. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press (2006).
3. Chemical Kinetics and Reaction Dynamics by Santosh K. Upadhyay, Anamaya Publishers, New Delhi, 2006.
4. Chemical Kinetics and Dynamics, J.I. Steinfeld, J.S. Francisco and W.L. Hase, 2nd Edition, Prentice Hall International, Inc., 1999.
5. Chemical Kinetics: From Molecular Structure to Chemical Reactivity, by L. Arnaut, Sebastiao Formosinho, Hugh Burrows, Elsevier, 2007.

M.Sc. CHEMISTRY
SEMESTER - III

MCH-316 Paper No :XV(iv)	QUANTUM CHEMISTRY	Theory (Marks)		Total Credits (Marks)
		U.E(60)	I.A(40)	03 (100)

Objective: The unit deals with the basic Concepts of Quantum Chemistry

Unit I Some Exactly Solvable Problems

Postulates of Quantum Mechanics. Discussion of the solution of the Schrödinger equation to some model systems viz. free particle, the rigid rotor, the harmonic oscillator and the hydrogen atom (derivation only of eigenvalue in last two problems. The method to find the wave function is only sketched and result is given). Simple discussion of potential barrier (short study). **15 L**

Unit II: Approximate Methods

The Variation theorem, linear variation principle. Time independent Perturbation theory (first order and non-degenerate), second order change of energy non-degenerate (withoutproof). Applications of variation method and perturbation theory to Helium atom. Only abrief sketch of time dependent perturbation theory. Formula of the Golden rule written down (without proof). Some simple applications indicated (without proof). **11 L**

Unit III: Angular Momentum, Spin and Electronic Structure

Angular momentum operators, Eigen values and eigen functions, addition of angular momenta, 6j and 9j symbols (without proofs), spin, Antisymmetry and Pauli Exclusion Principle. Electronic configuration, atomic state, Russell-Saunders coupling schemes, term separation energies of the pn configuration, magnetic effects; spin orbit coupling and Zeeman splitting, introduction to the method of self-consistent field. **12 L**

Unit IV: Molecular Orbital Theory

Hybridization & valence MO's of H_2O, NH_3 and CH_4. Huckel Molecular Orbital Theory of conjugated systems. Delocalization energy, electron density, bond order. Application of HMO to ethylene, butadiene, cyclopropenyl radical & benzene (only qualitative discussion forbenzene). **10 L**

Essential Reading

1. L. Levine, Quantum Chemistry 5th Ed. Prentice Hall Inc. New Jersy(2000).
2. T. Engel and P. Reid, Physical Chemistry, Published by Pearson Education and Dorling Kindersley (India)(2006).
3. Donald A. McQuarrie, Quantum Chemistry, Oxford University Press, 1983 (541.28MCQ).
4. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill Publishing Company New Delhi.
5. Eyring, Walter & Kimball, Quantum Chemistry, John Wiley & Sons, Inc., Chapman & HallLtd, 1946.

M.Sc. CHEMISTRY
SEMESTER - III

Practical Course Work

PHYSICAL CHEMISTRY PRACTICAL-III MCHPL	Practical (Marks)		Total Credits (Marks)
	UE (60)	IA (40)	04 (100)

S.No **EXPERIMENT**

1. Determine the molecular weight of the given polymer sample by viscosity method.
2. Determine the ionization constant of acetic acid by conductivity method.
3. Titrate using conductometer a moderately strong acid (salicylic/mandelic acid) by the
   (a) salt-line method
   (b) double alkali method
4. Titrate a mixture of copper sulphate, acetic acid and sulphuric acid against sodium hydroxide conductometrically.
5. Titrate a tribasic acid (phosphoric acid) against NaOH and Ba(OH)2 conductometrically.
6. Carry out the following titrations conductometrically:
   (a) Magnesium sulphate against $BaCl_2$ and its reverse titration
   (b) HCl versusNH_4OH
   (c) Sodium oxalate against HCl.
7. Determine the rate constant of saponification of ethyl acetate at different temperatures and calculate the energy of activation of the reaction by conductivity method.
8. Find out the rate constant of acid-catalysed hydrolysis of sucrose by polarimeter.
9. Study the rate equation for mutarotation of D-glucose in water using polarimeter.
10. To determine the partial molar volumes of sodium chloride in water by density measurements. (Page 30 - Das & Behra).
11. To find the formula of the copper - ammine complex ion in aqueous solutions by partition method. (Page 108 - Das & Behra)
12. To determine the hydrolysis constant of aniline hydrochloride by partition method. (Page 113 - Das & Behra)
13. Titrate phosphoric acid potentiometrically against sodium hydroxide.
14. Titrate potentiometrically solutions of
    (a) KCl/ KBr/KI;
    (b) mixture of KCl + KBr + KI and determine the composition of each component in the mixture.
15. Titrate potentiometrically a solution of ferrous ions against $KMnO_4$/ $K_2Cr_2O_7$. Carry out the titration in the reverse order
16. Determine the solubility and solubility product of an insoluble salt, AgX (X=Cl, Br or I) potentiometrically.
17. Determine the hydrolysis constant of aniline hydrochloride by pH meter.
18. Determine potentiometrically the heat of reaction equilibrium constant and other thermodynamic functions for a given reaction such as:
    $Zn + Pb^{++} \Leftrightarrow Zn^{++} + Pb$
19. Determine the mean ionic activity coefficients of hydrochloric acid solutions at different concentrations by potentiometer.
20. Determination of the temperature dependence of the solubility of a compound in two solvents having similar intermolecular interactions (benzoic acid in water and inDMSOwater mixture) and calculate the partial molar heat of solution.
21. Determine the transport numbers of cations and anions in a solution of its salt by moving boundary method.

M.Sc. CHEMISTRY
SEMESTER - III

22 To determine the degree of ionization of sodium chloride at different concentrations of its aqueous solutions from the depression of freezing point measurements.
(Page 45 - Das & Behra)

23 Estimation of Pb^{2+} and Cd^{2+}/Zn^{2+} and Ni^{2+} ions in a mixture of these ions by polarography.

24 Determination of dissolved oxygen in aqueons solution of organic solvents by polarography

25 Determine the formula and overall stability constant of lead oxalate complex at 25°C by polarographic method.

26 To determine the rate constant of the acid hydrolysis of acetal by dilatometry at 298.15k. (Das & Behra)

M.Sc. CHEMISTRY
SEMESTER - III

MCH-317 Paper No :XVI	CHEMISTRY OF SYNTHETIC AND NATURAL MATERIALS-I	Theory (Marks)		Total Credits (Marks)
		U.E. (60)	I.A. (40)	04 (100)

Objective: The unit deals with the basic concepts of Chemistry of various types of Advance Materials

Unit I: Superconductors

Superconductivity and its origin, High temperature superconductors, Miessner effect, London equation, Type I and II superconductors, Isotope effect, Penetration depth and Coherence length, Anisotropy, Heat capacity, Copper pairs, Josephson effect, BCS theory of superconductivity, Hysteresis in superconductors, Organic superconductors. **15 L**

Unit II: Chemical Biology

Introduction: What is Chemical Biology and how it differs from Biochemistry; Basics of Biology: Amino acids, and peptides, Sugars-their function and importance. What is PNA and how it differs from DNA and RNA, synthesis of PNA monomer, oligomer and its applications., Microscopy and Spectroscopy in Biology: AFM, SEM, TEM, DLS, ORD, CD, NMR, MS UV-Vis, Fluorescence **12 L**

Unit-III: Analytical Methods

Analytical Chemistry: Introduction, Classification of Different Analytical Techniques (chemical methods of analysis, electrical methods ofanalysis, optical methods of analysis, thermal methods of analysis). Criteria for Evaluating the Utility of Analytical Techniques. Evaluation of analytical data (errors, detection and minimization), accuracy, precision. Mean, median, mode, deviation, standard deviation, relative standard deviation, co-efficient of variation, precision, Gaussian distribution of data, t-test, Chi-square test. **15 L**

Unit-IV: Metal Complex Sensitizers

Concept of metal complex sensitizers; electron relay; metal colloidal systems; semiconductor supported metal oxide systems; nitrogen fixation; water photolysis; carbon dioxide reduction **12 L**

Essential Reading

1. Dobson, Gerrard & Pratt, Foundations of Chemical Biology; Oxford Univ. Press;2002.
2. Miller & Tanner, Essentials of Chemical Biology: Structure and Dynamics of BiologicalMacromolecules; Wiley; 2002.
3. Solid State Physics by Lovel , Avery and Vernon

Suggested Reading

1. Waldman & Janning, Chemical Biology: A Practical Course; Wiley- VCH;2004.
2. Joseph R. Lackowicz, Principles of Fluorescence Spectroscopy; Springer;2006.

M.Sc. CHEMISTRY
SEMESTER - III

MCH-318 Paper No :XVII	ENVIRONMENTAL AND GREEN CHEMISTRY	Theory(Marks)		Total Credits (Marks)
		U.E. (60)	I.A.(40)	04 (100)

Objective: The unit deals with the basic concepts of Environmental and Green Chemistry

Unit I: Water Chemistry **15 L**

Water-quality parameters and standards: Physical and chemical parameters, Dissolved oxygen, BOD, COD, Total organic carbon (TOC), Total nitrogen, Total sulfur, Total phosphorus and Chlorine.

Chemical Toxicology: Toxic chemicals in the environments, Impact of toxic chemicals on enzymes, Biochemical effects of arsenic, chromium, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur oxides.

Unit II: Novel Inorganic Solids

Synthesis and modification of inorganic solids: Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods. **12 L**

Inorganic solids of technological importance: Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – colored solids, white and black pigments. Molecular material and fullerides, molecular materials and chemistry – one-dimensional metals, molecular magnets, inorganic liquid crystals.

Unit III: Nanomaterials

Overview of nanostructures and nanomaterials: classification. Preparation of gold and silver metallic nanoparticles, self-assembled nanostructures-control of nanoarchitecture-one dimensional control. Carbon nanotubes and inorganic nanowires. Bio-inorganic nanomaterials, DNA and nanomaterials, natural and artificial nanomaterials, bionano composites. **10 L**

Unit IV: Green Chemistry

Introduction. Need for Green Chemistry, Goals of Green Chemistry, Limitations/ Obstacles in the pursuit of the goals of Green Chemistry, Principles of Green Chemistry and Designing a Chemical synthesis. **15 L**

Future Trends in Green Chemistry: Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; crystal controlled solid state synthesis; Green chemistry in sustainable development.

Suggested Books

1. Colin Baird, Environmental Chemistry, W.H. Freeman and Company, New York (1995).
2. A.K. De, Environmental Chemistry, 4th Edition (2000), New Age International Private Ltd., New Delhi.
3. S.M. Khopkar, Environmental Pollution Analysis, 1st Edition (1993), Wiley Estern Ltd., New Delhi.
4. S.K. Banerji, Environmental Chemistry, 1st Edition (1993), Prentice-Hall of India, New Delhi.
5. G. J. Ferraudi, Elements of Inorganic Photochemistry, John Wiley & Sons (1988).
6. Matlack, A.S. Introduction to Green Chemistry, Marcel Dekker (2001).
7. Ahluwalia, V.K. & Kidwai, M.R. New Trends in Green Chemistry, Anamalaya Publishers (2005).
8. Ryan, M.A. & Tinnesand, M. Introduction to Green Chemistry, American Chemical Society, Washington (2002).
9. Lancaster, M. Green Chemistry: An Introductory Text RSC Publishing, 2nd Edition, 2010.

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-401 Paper No :XVIII (i)	CHEMICAL APPLICATIONS OFGROUP THEORY	Theory (Marks)		Total Credits (Marks)
		U.E.(60)	I.A.(40)	03 (100)

Objective: Introduction to Advance Concepts in Group Theory and their Applications

Unit I: Symmetry Aspects of Molecular Vibrations **12 L**

Introduction, the symmetry of normal vibrations. Determining the symmetry types of the normal modes (Normal mode analyses of water molecule, carbonate ion and N_2F_2). Contribution of particular Internal Coordinates to normal modes. Symmetry selection rules for fundamental vibrational transitions (Qualitative treatment). The symmetry of group vibrations (a discussion of molecule $Cl_3C\text{-}CH_2\text{-}CCl_3$ to demonstrate vibrational modes of CH_2 group). Use of symmetry considerations to determine the number of active infrared and Raman lines (example SF_4).

Unit II: Symmetry Aspects of Hybrid Orbitals

Transformations properties of atomic orbitals. Hybrid orbitals for sigma bonds in trigonalplanar (BCl_3), tetrahedral (CH_4), square planar $[PtCl_4]^{2-}$ and trigonal bipyramidal (PF_5). Hybridization scheme for pi bonding in trigonal planar (AB_3) and tetrahedral (AB_4) systems. **12 L**

Unit III: Hybrid Orbitals as Linear Combination of Atomic Orbitals **14 L**

Mathematical form of equivalent and non-equivalent hybrid orbitals. Trigonal planar sp^2 equivalent hybrids in BCl_3; Tetrahedral sp_3 equivalent hybrid orbitals in CH_4 and trigonal bipyramidal dsp_3 non-equivalent hybrid orbitals in PF_5.

Unit IV: The Huckel Molecular Orbital Treatment and Symmetry Simplifications **12 L**

The LCAO method and secular equation. The simple Hückel approach in constructing and solving secular determinants for conjugated systems (ethylene, allyl system and butadiene), delocalization energies. Symmetry simplifications of Hückel Molecular Orbitalmethod (symmetry factoring of secular equation: 1,3- butadiene). Calculations of electron density, charge density, Bond order and free valence index.

Essential Reading

1. Chemical Applications of Group Theory: by F.A. Cotton.
2. Group Theory and Symmetry in Chemistry: by Lowell H. Hall
3. Symmetry, Orbitals and Spectra: by Milton Orchin and H.H. Jaffe.
4. Physical Methods in Chemistry: by R.S. Drago.
5. Molecular Spectroscopy: by G.M. Barrow, McGraw-Hill.

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-402 Paper No :XIX (i)	STEREOCHEMISTRY AND METAL ION CATALYSIS	Theory (Marks)		Total Credits (Marks)
		UE(60)	IA(40)	03 (100)

Objective: Introduction to Advance concepts in Stereochemistry and Metal ion catalysis

Unit I: Stereochemical Changes in Octahedral Complexes-I **12 L**

Outer sphere orientations, reactions of geometrical and optical isomers SN^1 dissociation or SN^2 displacement mechanisms, stereochemistry of the acid and base hydrolysis of Co(III) complexes, optical inversion reactions of some Co(III) complexes.

Unit II: Stereochemical Changes in Octahedral Complexes-II **12 L**

Isomerization reactions of octahedral complexes, recimerization of octahedral Co(III) complexes, salt, salt and solvent effects, photorecimization.

Unit III: Photochemical Reactions

Introduction, types of excitation, fate of excited molecules, quantum yield, types of photochemical reactions. **14 L**

Unit IV: Metal Ion Catalysis

Metal ion catalysis in acid-base reactions-hydrolysis, aldol condensation, carboxylation and decarboxylation, Metal ion catalysis in redox reactions, autoxidation of organic substances. **12 L**

Essential Reading

1. Inorganic Reaction Mechanism - F. Basolo & G. Pearson.
2. Inorganic Reaction Mechanism - J. O. Edwards
3. Langford, H. & Gray, H.B. *Ligand Substitution Processes* W.A. Benjamin

Suggested Reading:

1. Selected Topics in Inorganic Chemistry- Malik, Madan &Tuli.
2. Katakis, D. & Gordon, G. *Mechanism of Inorganic Reactions* John Wiley & Sons: N.Y. (1987).

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-403 Paper No: XX (i)	ORGANOMETALLIC CHEMISTRY-II	Theory (Marks)		Total Credits (Marks)
		U.E. (60)	I.A.(40)	03 (100)

Objective: Introduction to Advance concepts in Organometallic chemistry

Unit I: Fluxionality and Dynamic Equilibria **12 L**

Stereo-chemical non-rigidity in organometallic complexes. Scrambling of carbonyl groups in metal carbonyl complexes. Fluxionality and dynamic equilibria in olefinic, π-allyl and cyclopentadienyl complexes. Ring whizzing. Davies-Green-Mingo (DMG) Rules.

Unit II: Distinctive organometallic Reactions

Oxidative addition reactions (d^{10}, d^8 and d^7 complexes), Intramolecular oxidative addition reactions, C-H activation, cyclo-metallation and ortho-metallation, oxidative coupling reactions. Reductive elimination reactions (mono & binuclear systems), and β-elimination reactions, β-hydrogen elimination / β-hydrogen transfer reactions. Insertion reactions, insertion of carbonyls and alkene sand migratory insertion reactions. **12 L**

Unit III: Compounds of Transition Metal-Carbon Multiple Bonds **14 L**

Transition metal carbenes, Fischer carbene & Schrock's carbenes their requisites and properties, Tebbe's reagent. Intermediate carbenes between Fischer & Schrock carbene, Grubb's catalyst Ist & 2nd generation catalyst and its applications. Transition metal carbyne complexes, their preparation properties and structures.

Unit IV: Industrial Applications of Organometallic Complexes **12 L**

Catalytic applications of organometallic complexes. Alkene hydrogenation and Wilkinson catalyst. Synthesis gas (H_2/CO) formation. Monsanto –Acetic acid process. Hydroformylation reactions. Wacker Oxidation process and isomerization. Polymerization and Ziegler-Natta catalysis.

Essential Reading

1. Metallo-organic Chemistry- Anthony J Pearson, John Wiley & Sons Inc,(1985).
2. Inorganic Chemistry – Principles of Structure & Reactivity, J E Huheey, Elllen A Keiter& Richard L Keiter, IV Edition (2005).
3. Introduction tom metal n-complex chemistry- M. Tsutsui, M.N. Levy, A. Nakamura, M.Ichikawa and K. Mori, Plenum Press, New York I Heme(1970).
4. Organometallic Chemistry - R. C. Mehrotra &A. Singh, Wiley Eastern Ltd.(2000).
5. Advanced Inorganic Chemistry - F.Albert Cotton, Geoffrey Wilkinson, Carlos A Murillo & Manfred Bochmann, VI Edition, John Wiley & Sons Inc(1999).

Suggested Reading:

1. Infrared and Raman spectra of Inorganic & Coordination Compounds; Kazuo Nakamoto, IV Edition, John Wiley & Sons Inc (1986).
2. Chemistry of the elements, N.N. Greenwood and A. Earnshaw, Pergamon.
3. Compressive coordination chemistry Eds.: G. Wilkinson, R.D. Gillards and J.A. McCleverty, Pergamon

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-404 Paper No :XXI (i)	BIO-INORGANIC CHEMISTRY–II	Theory (Marks)		Total Credits (Marks)
		U.E(60)	I.A(40)	03 (100)

Objective: Introduction to Advance concepts in Bioinorganic Chemistry

12 L

Unit I: Metallo-Proteins

Biological ligands for metal ions: Macrocycle, nucleobase, nucleotides and nucleic acids, coordination of metals by protein. Heme and nonheme protein, oxygen uptake, structure and function of haemoglobin, myoglobin, hemocyanin, hemerythrin.

Unit II: Metallo-enzyme **12 L**

Principle involved and role of various metals viz. Zn, Fe, Cu and Co; carboxy peptidase, carbonic anhydrase, Alcohol dehydrogenase, Zinc Fingers, other gene regulatory Zinc proteins, cobalomine, mutase activities of coenzyme B_{12}.

14 L

Unit III: Iron-Sulfur and other Non-Heme Proteins

Rubredoxine Structure and function of iron sulphur protein, cytochromes, cytochrome P-450,oxygen transfer long distance electron transfer.

Unit IV: Application of Bioinorganic Chemistry **12 L**

Medicinal and therapeutic; metal deficiency and disease, toxic effect of metals, metals used fordiagnosis and chemotherapy, gold compound as Anti-Rheumatic agent. Nitrogen cycle; biological nitrogen fixation, metalloenzyme in biological nitrogen cycle, molybdenum nitrogenase, other nitrogenase model

Essential Reading

1. Principles of Bioinorganic Chemistry S.J. Lippard and J. M. Berg, University Science Books.
2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J. S. Valentine, UniversityScience Books.
3. Inorganic Biochemistry, Vols. I and II, Ed. G. L. Eichhorn, Elsevier.

Suggested Reading:

1. Progress in Inorganic Chemistry, Vols. 18 and 38, Ed. J.J. Lippard, Wiley.
2. Inorganic Chemistry, James E. Huheey, Harper International, Sixth Edition (1983)..

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-405 Paper No :VIII (ii)	TECHNICAL CERAMICS	Theory (Marks)		Total Credits (Marks)
		U.E. (60)	I.A. (40)	03 (100)

Objective: Introduction to basic types in Ceramics materials and their applications

Unit I: Piezoelectric and Optoelectric Ceramics **8 L**

History of development, centrosymmetric and noncentrosymmetric (n.c.s.) crystals, polarization in n.c.s. crystals, piezoelectric ceramics, piezoelectric equations, definition of piezoelectric terms and their characteristics, poling of piezoelectric ceramics, dimensional changes, ferroelectric ceramics general features and applications.Electroptic ceramics (e.o.c): general aspects, birefringence in e.o.c. Optical phase retardation, generation of various colours, Electroptic coefficients r and R, mode of application of e.o.c., characteristics required in e.o.c., composition systems- role of donors, acceptors and isovalent additives, processing and fabrication; loop in e.o.c. special features, intermediate polarization state, different types of hyteresis loop; electrochemical properties, piezoelectric deformation (extended treatment); applications

Unit II: Ferrite Ceramics **12 L**

Magnetic ferrite- general aspects, ferromagnetic, anti-ferromagnetic ordering in spinels, site preference in spinels, Garnet, magnetic moments and accupancy of A&B sites, various ferrite compositions and their magnetic properties. Processing of ferrites – extended treatment. Nonmicrowave ferrite compositions, theirB/H other characteristics, applications; microwave ferrites – characteristics and applications

Unit III: Ceramic Sensors **14 L**

General aspects, intrinsic and extrinsic conductors,.NTC thermistors- History of development; NTC device construction principle, device types and dimensions, electrical properties, resistivity temperature behaviour, stability and sensitivity of thermal sensors, time constant and dissipation constant. Device chemistry - - dependence of B and resistivity upon composition.Factors affecting sensor performance, stability and life resistance shift r on aging, thermophysical properties of thermistor materials. NTC sensor applications, PTC thermistors, History of development, general applications, PTC thermistors – electrical behaviour, resistivitytemperature relationship, other electrical parameters, V-1 curve-important features. Devicechemistry
– role of dopant, isovalent, altervalent and barrier layer modifiers, sintering aids, curie temperature control. Gas sensors- general aspects, self-generating galvanic type oxygen sensors, construction, special features; modulating type gas sensors - general aspects, material requirements , temperature dependence of resistivity,its control

Unit IV: Bioceramics **14 L**

Bioceramics, Bioinert versus Biocompatible Materials, Partially stabilized Zirconia, Carbons and Carbon- composite ceramics, Mica glass ceramics, Bioactive ceramics- Bioactive glass:bone bonding, Conventional Bioactive glasses, Sol- GEL routes to Bioactive glass, Problems of Longevity of implant use, Bioceramic composites, Composites based on HAP, Bone graft materials and applications.

Essential Reading:

1. Introduction to Fine ceramics by Noburu Ichinose (ed.) John Wiley and Sons., New York (1987)

M.Sc. CHEMISTRY
SEMESTER - IV

2. Ceramic Materials for Electronics – R.C. Buchanan (ed.) Marcel Deller, New York(1991)
3. Chemical Processing of Ceramics by Burtrand I. Lee, Edward J. A. Pope (ed) Marcel Deller,NewYork
4. Chemistry of Advanced Materials, an overview (ed) By Leonard V. Interrante, Mark JHampden –Smith, John Wiley and Sons., New York Marcel Deller,New York

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-406 Paper No:XIX(ii)	PROCESSING AND CHARACTERIZATIONOF CRYSTAL STRUCTURES	Theory (Marks)		Total Credits (Marks)
		U.E. (60)	I.A. (40)	03 (100)

Objective: The paper comprises of the techniques used to grow thin films and the characterization of solid state materials using different spectroscopies

Unit I: Preparation of Thin Films of Crystals **12 L**

Electrochemical methods**:** anodic oxidation, cathodic deposition, electro-less deposition**.** Chemical method: chemical vapour deposition, sol gel method, Langmuir Blodgett, photolithography Physical methods: cathode sputtering, magnetron sputtering, vacuum evaporation, molecular beam epitaxy, Application techniques: spin coating, flow coating dip coating and printing (screen printing, gravure printing, flexo printingand ink jet printing

Unit II: Preparation of Solid Solutions **10 L**

General concepts on the requirement solid solution formation, substitution solid solutions, interstitial solid solution, Mechanism of complex solid solutions, Creation of cation, anion vacancies creation of interstitial of cations and anions, double substitution, experimental techniques for studying solid solutions

Unit III: Characterization of Crystals Structures **12 L**

X-ray techniques: X-ray diffraction and Bragg Law, Diffraction under ideal and non-ideal condition, X-ray scattering and structure factor, X-ray diffractometer, X-ray data file analysis, Chemical analysis by emission (x-ray fluorescence), X-ray absorption techniques (AEFS,EXAFS)Single crystal X-ray diffraction ,different cameras and their special features Electron spectroscopic techniques; principles, instrumentation, data analysis and applications of UPS.XPS, AES , Electron loss energy spectroscopy, neutron diffraction

Unit IV: Electron Microscopic and Thermal Characterization of Crystals Structures **14 L**

Scanning Electron Microscopy – basic principle, instrumentation, electron specimen interaction, topographical and atomic number contrast, Transmission Electron Microscopy; practical aspect of microscopy, amplitude and phase contrast imaging, kinematical theory of image contrast, electron diffraction. Atomic Force Microscopy: basic principles, Atomic Force Microscopy modes, phase imaging, face curve, application of Atomic Force Microscopy; Thermal techniques: principles, instrumentation, data analysis and applications of DSC, TGA, DTA and their special features

Essential Reading:

1. Introduction to Materials Chemistry by H.R. Allcock Wiley.
2. Elements of X-Ray Diffraction (3rd Edition) by B. D. Cullity and S.R. Stock
3. Introduction to X-Ray Powder Diffractometry by Ron Jenkins and Robert Snyder.

Suggested Reading

2. Understanding solids: The science of materials by Richard Tilley(Wiley).
3. Scanning and Transmission Electron Microscopy: An Introduction by Stanley L. Flegler,
4. John W. Heckman Jr., and Karen L. Klomparens

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-407 Paper No: XX (ii)	POLYMER TECHNOLOGY, PROCESSING AND SPECIALITY POLYMERS	Theory (Marks)		Total Credits (Marks)
		U.E. (60)	I.A.(40)	03 (100)

Objective: The paper deals with the study of polymer processing techniquesand some specialty polymers

Unit I: Polymer Technology – II

Additives for Plastics: Fillers, Plasticizers, Stabilizers, Lubricants, Flame Retardants, Foaming Agents, Crosslinking Agents, Manufacture, Properties and Applications of Major Thermoplastics and Thermosetting Polymers: PE, PP, PVC, PS, Polyamides, Polyesters, Phenolic Resins, Amino Resins and Epoxy Resins, Polymeric Coatings **10 L**

Unit II: Unit II: Polymer Processing

Classification of Polymer Processing, Simple Model Flows for Analyzing Processing Operations with Examples, Extrusion and Extruders, Calendaring, Film Blowing, Injection Molding, Blow Molding, Rotational, Transfer and Compression Molding, Vacuum Forming, Reaction Injection Molding **10 L**

Unit III: Biopolymers

Structure, Functions and Properties of Naturally Occurring Polymers such as Proteins, Polysaccharides and DNA, Polymer Chemistry of Biological Processes, Synthetic Biopolymers, their Fabrication and Applications **14 L**

Unit IV: Specialty Polymers

Conductive Polymers: Theory of Conduction, Synthesis and Applications of Conductive Polymers, Biodegradable Polymers, Biomaterials, Polymers in Medicine, Drug Delivery Systems, Recycling of Polymers **12 L**

Essential Reading:

1. Text Book of Polymer Science By F. W.Billmeyer
2. Introduction to Polymers by R. J. Young and P. A.Lovel
3. Polymer Chemistry by G.Challa

Suggested Reading:

1. Polymers: Chemistry and Physics of Modern Materials by JMG Cowie
2. Principles of Polymerization by George Odian

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-408 Paper No :XXI (ii)	PROPERTIES OFMATERIALS	Theory (Marks)		Total Credits (Marks)
		U.E(60)	I.A(40)	03 (100)

Objective: The paper focuses on the properties of materials and their common applications

Unit I: Electronic State in Solids **12 L**

Free electron theory of standing and running waves, density of state, band theory, K. space and Brillouin zones, band structures of metals, insulator and semiconductors, the concept of hole, extrinsic (impurity) semiconductors, Fermi energy, position of Fermi level, free carrier concentration in intrinsic and extrinsic semiconductors, application of semiconductors, application of semiconductors, I-VI compounds, I -IV compounds,III-V compounds

14 L

Unit II: Electrical Properties

Introduction, electron drift in an electrical field, relaxation time and mean free path, electrical conductivity of non-degenerate and degenerate gases , specific conductance of conductor, Widemann-Franz-Lorentz law, electrical conductivity of metals and alloys., piezoelectric materials temperature dependence carrier mobility, electrical conductivity of pure metal, electrical conductivity of alloys. **10 L**

Unit III: Magnetic Properties

Introduction: Classification of magnetic materials, diamagnetism, paramagnetic, ferromagnetic anisotropy, ferromagnetic domains, origin of domain wall antiferromagnetism, antiferromagnetic, domains, ferrimagnetism, normal spinel's inverse spinels, ferromagnetic domain. **10 L**

Unit IV: Optical Properties

Introduction: Refractive index, dispersion, absorption birefringence, photoluminescence laser, nonlinear optical materials- non-linear optical effect, second and third order molecular hyper polarisability and second order electric susceptibility materials for second and third order harmonic generation.

Essential Reading:

1. Solid state physics by Epifanov.
2. Materials Science by Anderson and lever.

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-409 Paper No :XVIII (iii)	MEDICINAL CHEMISTRY ANDBIOMOLECULES	Theory (Marks)		Total Credits (Marks)
		UE(60)	IA(40)	03 (100)

Objective: The paper comprises of Medicinal Aspects of Organic chemistry and Biomolecules

UNIT- I: Drug design

Concept of lead compound, lead modification, prodrugs and soft drugs, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism, spatial considerations. Occupancy theory, rate theory, induced fit theory. Concepts of drug receptors. Free-Wilson analysis, Hansch analysis, relationship between Free-Wilson and Hansch analysis. LD-50, ED-50 (Mathematical derivations of equations excluded). **8 L**

UNIT-II: Antibiotics, cardiovascular and local anti-infective drugs **12 L**

Cell wall biosynthesis, inhibitors, β-lactam rings, antibiotics inhibiting protein synthesis. Synthesis of Penicillin G, Ampicillin, Tetracycline, Ciprofloxacin, Norfloxacin, dapsone. Cardiovascular diseases, drug inhibitors of peripheral sympathetic function, central intervention of cardiovascular output. Direct acting arteriolar dilators. Synthesis of amylnitrate, sorbitrate, diltiazem, quinidine, verapmil, and oxyprenolol.

Unit III: Psychoactive Drugs - The Chemotherapy of Mind

Introduction, neurotransmitters, CNS depressants, general anaesthetics, mode of action of hypnotics, sedatives, anti-anxiety drugs, benzodiazepines, buspirone, neurochemistry of mental diseases. Antipsychotic drugs – the neuroleptics, antidepressants, butyrophenones, sernndipity and drug development, stereochemical aspects of psychotropic drugs. Synthesis of diazepam, oxazepam, chlorazepam, alprazolam, phenytoin, ethosuximide, trimethadione, barbiturates, thiopental sodium, glutethimide. **08 L**

Unit IV: Antimicrobial Drugs

Quinolone, Mechanism of action, Non-benzoid nitro compounds, nitrofurans, parasitic diseases, Chemotherapy of malaria, 8 & 4-aminoquinolines, other antiprotozoal drugs, antifungal drugs Imidazole compounds, mechanism of action of imidazoles, antihelmintics, antiviral chemotherapy**.** **14 L**

Essential Reading

1. Introduction to Medicinal Chemistry, A. Gringauge, Wiley-VCH.
2. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Editedby J.N. Delgado and W. A. Remers, J.B. Lipincott Company.
3. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, AcademicPress.
4. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley & SonsLtd.

Suggested Reading

1. A Text Book of Medicinal Chemistry, Vol-I and Vol-II, Surendra N. Pandeya, SGPublishers.
2. An Introduction to Drug Design, S.S. Pandeya and J. R. Dimmock, New Age International Publishers.
3. Medicinal Chemistry, Ashutosh Kar, New Age InternationalPublishers.

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-410 Paper No:XIX(iii)	ADVANCED METHODS IN ORGANIC SYNTHESIS	Theory (Marks)		Total Credits (Marks)
		UE (60)	IA (40)	03 (100)

Objective: The unit will help students to understand the various tools used in Advance Organic Synthesis

Unit I Carbenes, Carbenoids and N-Heterocyclic carbenes (NHC)

Introduction, Fischer and Shrock carbenes with their synthetic applications. Dotz benzannulation reaction. The nature of N-heterocyclic carbenes: Synthesis (synthesis of the imidazolium salts and transition metal complexes of NHC) and properties (basicity of NHC, steric properties, and decomposition pathways of NHC). Reactions based on carbenes insertions into C-H, N-H, and O-H bonds. Ring closing metathesis (RCM), ring opening metathesis (ROM), enzyme metathesis (EM), ring-closing-ring-opening metathesis (RCM-ROM), cross metathesis (CM) and tandem metathesis. **12 L**

Unit II: Radical Chemistry:

Introduction, generation of radicals, addition to a pi-bond, fragmentation, atom abstraction (reaction with a sigma bond), radical-radical combination, disproportionation, electron transfer, addition of a nucleophile, and loss of a leaving group. Minisci reaction, Kagan-Molander coupling, Sandmeyer reaction, and Hunsdiecker reactions. **12 L**

Unit III: C-H Bond Functionalization/Activation:

Definition and challenges & logic of C-H functionalization, alpha C-H functionalization of ethers and alcohols, diastereo control in C-H methylene group, sp^2 C-H functionalization, activated sp3 C-H functionalization (allyl, benzyl, propargyl and carbonyl; alpha heteroatomic hydrogen), oxidative C-H functionalization, metalloporphyrin complex in C-H functionalization and other new particularly in the development of novel catalytic, methodologies for multiple C-H (sp^2, sp3) functionalization.. **08 L**

Unit IV: Multicomponent Reactions (MCRs):

History of multicomponent chemistry, The discovery of new isocyanide based multicomponent reactions, multicomponent reactions with carbonyl compounds, metal catalyzed multicomponent reactions and their applications: Hantzsch synthesis of dihydropyridines, Strecker synthesis of α-amino acids, The Biginelli reaction, Bucherer-Bergs reaction, Passerini reaction, Ugi reaction, and the Domino-Knoevenagel-Hetero-Diels-Alder reaction **14 L**

Essential Reading:

1. Kurti, L.and Czako, B. Strategic applications of Named reactions in organic synthesis(2004).
2. Carruthers, W. and Coldham, I. Modern methods of organic synthesis, Cambridge University Press (2004).
3. D'Souza D. M, Müller T. J. J. Multi-component syntheses of heterocycles bytransition-metal catalysis. Chem. Soc. Rev. 2007, 36:1095-1120.
4. Organometallic reagents in synthesis by Paul R. Jenkins.
5. N-Heterocyclic Carbenes in Transition Metal Catalysis by Frank Glorius, Springer-Verlag BerlinHeidelberg 2007.

Suggested Reading:

1. Organometallic-Chemistry- R.C. Malhotra & A. Singh, Wiley Eastern Ltd.(2000).
2. Bruckner, R. Advanced Organic Chemistry Elsevier(2002).
3. Clayden, Greeves, Warren & Wothers, Organic Chemistry Oxford University press(2001).
4. A.L. Lehninger, Principles of Biochemistry, W. H. Freeman & Co.USA.

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-411 Paper No :XX (iii)	CHEMISTRY OF NATURALPRODUCTS	Theory (Marks)		Total Credits (Marks)
		U.E(60)	I.A(40)	03 (100)

Objective: The unit will help students to understand the Chemistry of Natural products

Unit ITerpenoids:

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, synthesis of the following representative molecules: Citral, geraniol, α-Pinene, Camphor **12 L**

Unit II:Alkaloids:

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, synthesis and biosynthesis of the following: Ephedrine, Nicotine, Morphine. **12 L**

Unit III:Steroids:

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Androsterone, Testosterone, Estrone, Progestrone. **08 L**

Unit IV: Prostaglandins and Flavonoids:

Discuss about the structure Prostaglandins and Flavonoids. Occurrence, nomenclature and general methods of structure determinations, isolation and synthesis, Quercetin, Flavones, Flavonols. **14 L**

Essential Reading:

1. I.L. Finar, Organic chemistry, Vol. II, ELBS Publications, UK.
2. J. Mann, R.S. Devison, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, Naturalproductschemistry and biological significance, Longman Publisher, Essex,UK.
3. B.A. Bohm, Introduction to flavonoids, Harwood Acad. Publishers, USA.
4. Natural Products- Chemistry and Biological Significance, J. Mann, R.S. Davidson, J. B. Hobbs, D.V. Banthrope and J. B. Harborne, Longman, Essex.
5. Organic Chemistry Vol. II, I.L. Finar, ELBS. 3. Stereo selective synthesis- APractical Approach, M. Nogradi, VCH.

Suggested Reading

1. Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.
2. Chemistry, Biological and Pharmacological Properties of Medicinal Plants from the Americas, Ed. Kurt Hostettmann, M. P. Gupta and A.Marston, Harwood Academic Publishers.
3. Introduction to Flavonoids, B. A. Bohm, Harwood Academic Publishers.
4. New Trends in Natural Product Chemistry, Atta-ur-Rahman M. I. Choudhary, Harwood Academic Publishers.
5. Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-412 Paper No:XXI(iii)	APPLICATIONS OF SPECTROSCOPY	Theory (Marks)		Total Credits (Marks)
		U.E(60)	I.A(40)	03 (100)

Objective: The unit will help students to understand the applications of Spectroscopy to Organic molecules

Unit I UV-visible and IR Spectroscopy **12 L**

Basics, Ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes, aromatic and heterocycles, Fieser- Woodward rules for conjugated dienes and carbonyl compounds, and effect of solvent on electronic transitions. IR frequencies of alkanes, alkenes, alkynes, aromatic compounds, and for all other functional groups. Effects of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. Applications of UV- visible and IR spectroscopy in Organic chemistry**.**

Unit II: Applications of ^{1}H and ^{13}C NMR spectroscopy **12 L**

First-order and Non-first-order spectra, spin-spin interaction between two, three, four and five nuclei (first order spectra), factors effecting coupling constant "J",classification of spin system like AB, AX, AX_2, ABX, AMX, ABC, A_2B_2.Resolution and multiplicity of 13C NMR, 1H-decoupling, noise decoupling, broad band decoupling; Deuterium, fluorine and phosphorus coupling; un-decoupled, Proton decoupled, Off resonance, factors affecting chemical shifts. Structural applications of ^{1}H and ^{13}C-NMR.

Unit III: 2D NMR Techniques: **08 L**

General idea about two dimensional NMR spectroscopy, APT, INEPT, DEPT, Correlation spectroscopy (COSY)- Homo COSY (1H-1H), TOCSY, Hetero COSY (HMSC, HMQC, HMBC), Homo and Hetero nuclear 2D resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

Unit IV: Optical rotatory dispersion and circular dichroism **14 L**

Cotton effect, types of ORD and CD curves-similarities and difference between ORD and CD curves and their application to stereochemical problems; Octant rule and its application in structural studies, lactone sector and α-Halo keto rule**.**

Essential Reading:

1. Kemp, W, Organic Spectroscopy, W.H. Freeman &Co.
2. R. M. Silverstein, G. C. Bassler and T. C. Morrill, Spectroscopic Identification of Organic Compounds,John Wiley &Sons.
3. M. L. Martin, J. J. Delpeuch and G. J. Martin, Heyden, Practical NMR Spectroscopy, Spectrometric Identification of Organic Compounds, JohnWiley.
4. R. J. Abraham, J. Fisher and P. Loftus, Introduction to NMR spectroscopy, Wiley.
5. J. R. Dyer, Application of Spectroscopy of Organic Compounds, Prentice Hall.
6. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw Hill.
7. Organic Spectroscopy, Second Edition, W. Kemp, ELBS Macmillan, 1987 for RD and CD and ESR.

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-413 Paper No:XVIII(iv)	ADVANCED MOLECULAR SPECTROSCOPY	Theory(Marks)		Total Credits (Marks)
		U.E(60)	I.A (40)	03 (100)

Objective: The unit deals with the Physical Aspects of Spectroscopy

Unit I: Introduction to Molecular Spectroscopy

Time dependent perturbation. Einstein coefficients, Lambert-Beer's law. Integrated absorption coefficients. Transiton dipole moments and general selection rules based on symmetry ideas. Electronic Spectroscopy: Electronic spectroscopy of organic molecules- benzene, effect of substitution- pyridine, pyrimidine, pyrazine, methyl substitution. Vibronic analysis. **15 L**

Unit II: Vibrational Spectroscopy

Group theory and symmetry classification of normal modes of vibration. Normal coordinate analysis in Cartesian and internal coordinates of small molecules: BF_3, NH_3. Square planar, trigonal bipyramid, framework and cage molecules. Jahn-Teller distortions. **11 L**

Unit III: Magnetic Resonance Spectroscopy

Electronic Spin Resonance spectroscopy. Basic principles. Relaxation and Line Widths. Zero-field splitting and Kramer's degeneracy. Isotropic and anisotropic hyperfine coupling constants. Spin Hamiltonian, Spin densities and McConnell relationship. Fine splitting in triplet spectra. Applications of ESR spectroscopy: Structure determination, Interpretation of ESR spectra of simple organic radicals like benzene radical anion, naphthalene radical anion, toluene and o-, m- and p- xylene radical ions from HMO theory. Study of unstable paramagnetic species, Kinetic studies of electron transfer reactions. **10 L**

NMR Spectroscopy: Mechanism of spin-spin spin-lattice relaxations and quantitative treatment of relaxations. Quantum mechanical treatment of the AB system. Selection rules and relative intensity of lines.

Unit IV: Mossbauer and other Spectroscopic Methods

Principles of Mossbauer spectroscopy: Isomer shifts. Quadrupole and nuclear Zeeman splitting. Applications in structure determination. **09 L**

Photoelectron Spectroscopy: Basic principles of PES/ ESCA and Auger spectroscopy to the studyof surfaces.

Essential Reading

1. D. C. Harris & M. D. Bertolucci. Symmetry and Spectroscopy: An introduction to vibrational and Electronic Spectroscopy.Dover Publication: New York (1990).
2. D. M. Bishop. Group Theory and Chemistry. Clarendon Press: Oxford, U.K. (1973).
3. A. Carrington & A.D. Maclachlan, Introduction to Magnetic Resonance, Chapman & Hall, NY (1983).
4. J.E. Wertz and J.R. Bolton, Electron Spin Resonance, Elementary Theory and Practical Applications, Chapman and Hall, NY(1986).
5. R. Chang, Basic Principles of Spectroscopy, McGraw-Hill, 1971.
6. R.V. Parish, NMR, NQR, EPR, and Mössbauer Spectroscopy in Inorganic Chemistry, Ellis Horwood Series, 1990
7. C.L. Briant & R.P. Messmer, Auger Electron Spectroscopy, Treatise on Materials Science and Technoloy, Vol. 30,Academic Press Inc., 1988.

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-414 Paper No :XIX (iv)	NANO CHEMISTRY	Theory (Marks)		Total Credits (Marks)
		U.E (60)	I.A(40)	03 (100)

Objective: The unit deals with the Chemistry at Nanoscale

Unit I Fundamentals of Nanoscience and Nanotechnology **10 L**

Solid materials and their strength, Perspective of length, Nanomaterials, Nanoscience and Nanotechnology, Nanostructures in nature, Prime materials, Carbon nanostructures viz. Carbon nanotube (Single-walled and multi-walled), Fullerenes, Surface effects of Nanomaterials, Surface plasmon resonance, Quantum size effects.

Unit II: Applications of Nanomaterials **5 L**

Importance of Nanomaterials (Gold, Silver, Dielectric and Magnetic Oxide Nanoparticles), Some selected applications like, Nanomaterials in medicine, Nanomaterials for energy sector, Kinetic energy (KE) penetrators with enhanced lethality, High energy density batteries, Nanomaterials in Next-Generation Computer, Nanomaterials in catalysis and sensors, Nanomaterials for water purification, Nanomaterials in communication sector, Nanomaterials in food, Nanomaterials for the environment, Nanomaterials in automobiles, Nanomaterials in ceramics industry.

Unit III: Synthesis of Nanomaterials

Introduction, Nanomaterials synthesis, Top-Down and Bottom-Up Approaches, **15 L** Solvothermal synthesis, Hydrothermal synthesis, Reverse micellar/Micro-emulsion method, Reverse micelles works as nano reactor, Mechanism for nanoparticle synthesis inside the reverse micelles, Co-precipitation, Sol-Gel Method, Polymeric Precursor Method and Sono-chemical Methods.Theory, Experimental conditions, Kinetics of solid state reactions and molten–salt routes

Unit IV: Characterization of Nanomaterials **15L**

(a) X-Ray Diffraction Technique: Structure of nanomaterials, X-ray diffraction (XRD), The Laue method, The Rotating crystal method, The Powder method, Determination of grain size/crystallite size using X-ray line broadening studies (Scherrer's formula), Determination of crystallite size distribution using X-ray line shape analysis.

(b) Electron Microscopic Techniques: Principles of electron microscopy, Scanning Electron Microscopy (SEM), Strengths and limitations of Scanning electron microscopy, Energy dispersive X-ray analysis (EDX), Transmission Electron Microscopy (TEM), Atomic Force Microscopy (AFM) and Scanning Tunneling microscopy (STM).

(c) Dynamic Light Scattering (DLS) Studies: Principle, Theory and Methodology.

(d) BET Surface Area Studies: Principle, Theory and Methodology.

Essential Reading

1. Principals of Nanoscience and Nanotechnology, M. A. Shah and Tokeer Ahmad, Narosa Publications, 2010.
2. Nano Materials, B. Viswanathan, Narosa Publications, 2009.

3. Nano: The Essentials, T. Pradeep, Tata Mcgraw Hill, 2009.
4. Chemistry of Nanomaterials: Synthesis, Properties and Applications by C.N.R. Rao, A.Mullerand A. K. Cheetham (eds.), Wiley-VCH, Weinheim, 2004.
5. Nanoscale Materials by Luis M. Liz-Marzan and Prashant V.Kamat, Kluwer Academic Publishers (Boston),2003.
6. "Nanomaterials Chemistry: Recent Developments and New Directions", ed. by C.N.R. Rao,A. Muller & A.K. Cheetham (Eds.), Wiley-VCH, 2007

Suggested Reading

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1. Solid State Chemistry and its applications, Anthony R. West, John Wiley &Sons.
2. Physical Principles of Electron Microscopy: An introduction to TEM, SEM and AFM byR.F. Eqerton, Springer,2008.
3. Introduction to Atomic Force Microscopy, Paul E. West, Pacific Nanotechnology,USA.
4. Solid State Chemistry Techniques, A. K. Cheetham and Peter Day, Oxford SciencePublications.
5. Scanning Probe Microscopy and Spectroscopy, Ronald Weisendanger, Cambridge University Press.

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-415 Paper No:XX (iv)	ADVANCED PHYSICAL CHEMISTRY	Theory(Marks)		Total Credits (Marks)
		U.E(60)	I.A(40)	03 (100)

Objective: To impart advanced level knowledge about the thermodynamic principles of various biological macromolecules along within the concepts of Statistical Mechanics

Unit I: Fundamentals of Biological Macromolecules **15L**

Nature of Chemical bonds in biological systems: Forces responsible for molecular conformation, e.g., Hydrogen bonds, ionic/electrostatic interactions, van der waals interaction, hydrophobic interaction, stereo-chemical factors. Properties of water; Thermodynamic principles in biological systems; Properties and classification of amino acids; Structures of nucleic acids. Protein structure and function. Properties of nucleosides and nucleotides; compositions of nucleic acids.

Unit II: Conformational Analysis

Polypeptide chain geometries and internal rotational angles: Ramachandran plots; Molecular mechanics; Stabilizing interactions in biomolecules. Complexities in modelling macromolecular structure; Molecular mechanics; simulating macromolecular structure; energy minimization; Molecular Dynamics **12L**

Unit III: Biopolymer interactions and Non-equilibrium Thermodynamics in Biology

Non-covalent interaction, Electrostatic: dipole-dipole interaction, Dispersion force interaction, Hydrophobic interaction. Multiple Equilibria and various types of binding processes in biological systems. Thermodynamics of biopolymer solutions, Flory-Huggins model of macromolecular solvation, Osmotic pressure and Donnan membrane equilibrium. **10L**

Unit IV: Statistical Mechanics and Biomolecular simulations

Chain configuration of macromolecule, Random walk model and statistical distribution of end-to-end dimension. Calculation of average dimension of various chain structures. Conformational transitions: Helix-coil transition, Protein folding problem. Molecular mechanics and dynamics: Basic principles-molecular representations-force fields-atom-atom pair potentials - bond length and bond angle and torsion angle potential-van der Waals and electrostatic potential concepts of molecular dynamics-introduction to time-step integration algorithms and force fields. **15L**

Essential Reading

1. C. R. CANTOR & SCHIMMEL. BIOPHYSICAL CHEMISTRY VOLS 1-3,, W. H. FREEMAN (1980).
2. MICHEL DAUNE, MOLECULAR BIOPHYSICS: STRUCTURES AND DYNAMICS (OXFORD UNIV. PRESS)
3. THOMAS E. CREIGHTON, THE BIOPHYSICAL CHEMISTRY OF NUCLEIC ACIDS & PROTEINS (HELVETICA PRESS) (HELVETICA PRESS)
4. THOMAS E. CREIGHTON, THE PHYSICAL AND CHEMICAL BASIS OF MOLECULAR BIOLOGY
5. M.V. VOLKENSTEIN, MOLECULAR BIOPHYSICS (ACADEMIC PRESS)
6. BIOPHYSICS BY W.HOPPE W. LOHMANN, H. MARKL, H. ZIEGLER (SPRINGER)
7. Y. MOROI, MICELLE - THEORETICAL AND APPLIED ASPECTS, PLENUM PRESS, NEW YORK, 1992.

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-416 Paper No :XXI (iv)	ELECTROCHEMISTRY	Theory (Marks)		Total Credits (Marks)
		U.E. (60)	I.A. (40)	03 (100)

Objective: The unit deals with the advanced Concepts of Electrochemistry

Unit I: Electrode Kinetics **10 L**

Charge transfer under zero – field, charge – transfer under the influence of an electric field, two – way electron transfer, equilibrium exchange current – density, interface out of equilibrium, derivation of Butler–Volmer equation, Tafel plots, multistep electrode reactions.

Unit II: Electrolyte Solution : **12 L**

Structure of water, effect of an ion on the structure of water, solvation number, activity, activity coefficients and ion – ion interactions, physical significance of activity coefficient of an electrolyte, determination of mean ionic activity coefficient by freezing point depression and e.m.f. measurement methods, limiting law, electro – chemical potential. Derivation of Debye –Hückel – Onsager equation

Unit III: Transport Phenomena:

Diffusion coefficients, Fick's first law of steady – state diffusion, Fick's second law of non –steady state diffusion, relation between diffusion coefficient and mean free path, relation between thermal conductivity / viscosity and mean free path of a perfect gas, Einstein's relation between diffusion coefficient and absolute mobility of ions, Stokes – Einstein equation, Nernst – Einstein equation, Nernst – Planck flux equation. **11 L**

UNIT IV: Adsorption and Electrical Double Layer:

Electrical double layer, thermodynamics of electrified interfaces, derivation of electrocapillary equation, determination of charge density on electrode, electrical capacitanceof the interface. **12 L**

Electrical Double Layer Models: Structure of electrified interfaces (Electrical double layer models), Helmholtz –Perrin, Gouy – Chapman, stern, Graham – Devanathan – Mottwatts, Tobin, Bockris, Devanathan models.

Essential Reading

1. J. O. M. Blockris and A. K. N. Reddy : Modern Electrochemistry, Vol. 1 : Ionics, 2nd Ed., PlenumPress, New York,1998
2. J. O. M. Blockris and A. K. N. Reddy and M. Gamboa – Aldeco : Modern Electrochemistry, Vol.2A, Fundamentals of Electrodics, 2nd Ed. Plenum Press, New York, 2000.
3. A. J. Bard and L. R. Faulkner, Electrochemical Methods : Fundamentals and Applications, 2nd Ed., John Wiley & Sons, New York,2002

M.Sc. CHEMISTRY
SEMESTER - IV

MCH-417 Paper No:XXII	CHEMISTRY OF SYNTHETIC AND NATURAL MATERIALS-II	Theory (Marks)		Total Credits (Marks)
		U.E. (60)	I.A. (40)	04 (100)

Objective: The unit deals with the various concepts of Superconductors, Supramolecular ChemistryPhotochemistry and handling of different Chemicals

Unit I: Applications of High Tc Materials:

Applications of High Tc Superconductors; Superconductivity Application in Power System; high and low temperature superconductors and their preparation; Properties of High Tc Materials: anisotropy, penetration depth; SQUID Magnetometers; Superconducting IR Detectors; Superconductor based Microwave Devices; Josephson junctions; Application of Superconductors in imaging and diagnostics **15 L**

Unit II: Supramolecular Chemistry

Introduction, host-guest interactions**,** classification of host-guest compounds, intermolecular forces, nature of supramolecular interactions, molecular recognition, chiral discrimination, molecular receptors and design principles, template effect, cryptands, cyclodextrins, calixarenes, calix yrroles, crown ether, catenanes rotaxanes, molecular capsules, and molecular self-assembly **12 L**

Unit III: Advance Quantum mechanics

Review of quantum mechanics; Born Oppenheimer approximation; Slater codon rules; Hartree flock equation; Koopman and Brilloiun theories; Roothan equation; Gaussian basis sets **10 L**

Unit IV: Excited state of metal Complexes

Concept of excited states in metal complexes; Comparison with organic compounds; electronically excited states; charge transfer spectra; charge transfer excitations; methods for obtaining charge transfer spectra; metal complex sensitizers; electron relay; metal colloid system **15 L**

Essential Reading

1. Supramolecular Chemistry J. M. Lehn,Wiley-VCH
2. Supramolecular Chemistry: J. W. Steed, J. L. Atwood; JohnWiley2002
3. Principles and Methods in Supramolecular Chemistry; H-J Schneider, A Yatsimirsky; John Wiley,2000.
4. Chemical safety matters – IUPAC – IPCS, Cambridge University Press,1992.
5. 2. OSU safety manual1.01.

Suggested Reading

3. Waldman & Janning, Chemical Biology: A Practical Course; Wiley- VCH; 2004.
4. Joseph R. Lackowicz, Principles of Fluorescence Spectroscopy; Springer; 2006.

M.Sc. CHEMISTRY
SEMESTER - IV

IN-HOUSE PROJECT WORK

The students of Semester-IV shall be allotted Research based project work under the supervision of the concerned faculty member in the discipline. The entire project work shall include Literature Survey, Experimental Procedures, and Characterization of the synthesized Compounds followed by compilation of Results as Project dissertation work. They shall submit a project dissertation towards the semester end, which shall be evaluated by an external expert and internal examiners followed by the presentation/ viva voce.