Choice Based Credit System (CBCS)

JAMIA MILLIA ISLAMIA

(A CENTRAL UNIVERSITY)

FACULTY OF NATURAL SCIENCES

M.Sc. CHEMISTRY

(Effective from Academic Year 2019-20)

SYLLABUS OF COURSES TO BE OFFERED

Core, Elective 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 practicals to be taken up by the students in every semester is provided in the course outline table along with the credits. In all semester, the Core papers are of 3 credits each (100 marks) consisting of university exam (UE) (75 marks) and internal assessment (IA) (25 marks). During the first two semesters, the practical course work carries one Credits (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 to be carried out in the last semester is worth 4 credits (200 marks). 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	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 and Photochemistry	03 (100)
Practical (Core)		MCH-203L	Organic ChemistryPractical-II	01 (50)
Theory (Core)	IX	MCH-204	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	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)**
Elective	**XVI**	**MCH-317**	**Chemistry of Synthetic and Natural Materials-I**	**04 (100)**
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				**04 (200)**

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)
Elective Paper	XVI	MCH-317	Chemistry of Synthetic and Natural Materials-II	04 (100)
Ability Enhancement	XVII	MCH-318	Environmental and Green Chemistry	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				04 (200)

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)
Elective	XVI	MCH-317	Chemistry of Synthetic and Natural Materials-I	04 (100)
Ability Enhancement	XVII	MCH-318	Environmental and Green Chemistry	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				04 (200)

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

PHYSICAL CHEMISTRY

SEMESTER-III

Theory (Core)	XII (iv)	MCH-313	Nuclear and Analytical Chemistry	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)
Elective	XVI	MCH-317	Chemistry of Synthetic and Natural Materials-I	04 (100)
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				04 (200)

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 (75)	I.A (25)	03 (100)

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

12 L

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.

Unit II: Non–Aqueous Solvents **12 L**

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 SO2.

14 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.

Unit IV: Inorganic Materials **12 L**

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.

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.

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SEMESTER - I

Suggested Reading

1. Mabbs, F. E. & Machin, D. J. *Magnetism and Transition Metal Complexes* Chapman andHall: 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).

Practical Course Work

MCH-101L	INORGANIC CHEMISTRY PRACTICAL -I	Theory (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 GrawHill.
3. Handbook of Preparative Inorganic chemistry Vol. I and II, Academic press.
4. Standard methods of chemical analysis by W.W. Scaff, Technica lPress.
5. Vogel's Qualitative Inorganic Analysis (revised), Orient Longman.
6. Vogel's textbook of quantitative Inorganic Analysis (revised).

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MCH-102 Paper No: II	ELEMENTS OF MATERIALS CHEMISTRY-I	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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 **14 L**

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

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

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SEMESTER - I

Suggested Reading:

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

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

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MCH-103 Paper No: III	STEREOCHEMISTRY & REACTIVE INTERMEDIATES	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	03 (100)

Objective: The unit comprises of Isomerism, Aroaaticity, Conformational Analysis and Reactive Intermediates 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,

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Suggested Reading

1. Organic Reactions, Stereochemistry and Mechanisms; P.S. Kalsi, Fourth edition, NewAge International Publishers,(2006).
2. Eliel, E. L. Stereochemistry of Carbon Compounds Textbook Publishers2003.
3. Bruckner, R. Advanced Organic Chemistry Elsevier(2002)

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 storageof solvents, thin layer chromatography and column chromatographyetc.
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.

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MCH-104 Paper No: IV	THERMODYNAMICS	Theory(Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	03 (100)

Objective: The unit deals with the Advance Concepts of Thermodynamics

Unit I Basic Thermodynamics **9 L**

Brief description of the laws of thermodynamics, Concepts of Entropy and Residual Entropy, Free energy and its Temperature dependence, Thermodynamic Equilibria and Free Energy Functions, Physical Equilibria Involving Phase Transitions, Thermodynamic Maxwell Relations.

Unit II: Equilibrium Thermodynamics **12 L**

Partial molar quantities: Partial molar free energy, Partial molar volume and Partial molar heat content and their 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, Non-ideal systems: Excess functions for non-ideal solutions. Gibbs Duhem Margules equation and its applications.

Unit III: Non Equilibrium Thermodynamics **10 L**

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, Chemical Reactions, Coupled Reactions and Electro-kinetic Phenomena.

Unit IV: Statistical Thermodynamics **14 L**

Concept of distribution, Thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition function - Translational, Rotational, Vibrational and Electronic partition functions, calculation of thermodynamic properties in terms of partition function. Applications of partition functions. Heat capacity behaviour of solids - Chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law and applications to metal. Bose-Einstein statistics - distribution law and application to helium

Essential Reading

1. An Introduction to Chemical Thermodynamics, R. P. Rastogi and R. R. Mishra, Vikas Publishing House Pvt. Ltd.
2. Physical Chemistry, P. W. Atkins, ELBS.
3. Statistical Thermodynamics (Hardback) By (author) M.C. Gupta, Publisher: New Age International.
4. Thermodynamics, J. Rajaram and J.C. Kuriacose, Educational Publishers.

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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. Statistical Mechanics, Donald A. McQuarrie, Viva Books Pvt. Ltd. New Delhi, 2003 (530.13 MCQ 270916)
5. Elements of Statistical Thermodynamics (2nd Edition), Leonard K. Nash, Addison Wesley, 1974. (541.369 NAS X639)
6. Physical Chemistry, *Statistical Mechanics*, Horia Metiu, Taylor & Francis, 2006 (530.13 MET 276461)
7. Statistical Thermodynamics, B.J. McClelland, Chapman and Hall & Science Paperbacks, London, 1973 (536.7 MCC 37251)

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

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SEMESTER - I

MCH-105 Paper No: V	GROUP THEORY AND SPECTROSCOPY	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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 C2V and C3V point groups (Construction not required). Representation reducible and irreducible, analysis of reducible representation. Simple Applications of the character table.

Unit- III: Electronic Spectroscopy fundamentals

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. **10 L**

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

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MCH-201 Paper No: VI	INORGANIC CHEMISTRY-II	Theory(Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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 **12 L**

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

Unit II: Stereochemistry and Bonding in Main Group Compounds **10 L**

VSEPR, Walsh diagram (tri- and penta atomic molecules), dπ-pπ bonds, Bent rule and energetic of hybridization, simple reactions of covalently bonded molecules.

08 L

Unit III: Unit III: Isopoly and Heteropoly Acids and Salts

Isopolymolybdates, isopolytungstate, isopolyvanadates, heteropoly anions, organo heteropolyanions and Heteropoly blues.

Unit IV: Metal Clusters **12 L**

Higher boranes, carboranes and metalloboranes, compounds with metal –metal multiple bonds metal carbonyls and halide clusters.

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Practical Course work

MCH-201L	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.

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MCH- 202 Paper No: VII	ELEMENTS OF MATERIALS CHEMISTRY-II	Theory(Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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 andFontana
2. Material Science and Engineering byRaghavan
3. Solid state Chemistry byA.R.West
4. Introduction to Polymers by R. J. Young and P. A.Lovell

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Suggested Reading:

Introduction to Solid State Chemistry A.R.West

5. Materials Science and Engineering: An Introduction, W.D. Callister,Wiley
6. Text Book of Polymer Science by F. W.Billmeyer
7. Principles of Polymerization by G.Odian
8. Polymer Science and Technology of Plastics and Rubbers by P.Ghosh

Practical Course work

MCH-202L	ELEMENTS OF MATERIALS CHEMISTRY PRACTICAL -II	Practical (Marks)		Total Credits
		U.E (25)	I.A (25)	01 (50)

S. No	Experiment
1.	To prepare polymethylmethacrylate by bulk method and determine its % yield and solubility.
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 preparae 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 manusla prepared byTeacher-In-charge
2. A laboratory Manual of Metals and Alloys by S.M. Asharaf, Sharif Ahmad and UfanaRiaz
3. A laboratory Manual of Polymers by S.M. Asharaf, Sharif Ahmad and UfanaRiaz

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MCH-203 Paper No: VIII	PERICYCLIC REACTIONS AND PHOTOCHEMISTRY	Theory(Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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.

Unit III: Basics and Photochemistry of Aromatic Compounds **10 L**

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.

Unit IV Photochemistry of Alkenes and Carbonyl Compounds **14 L**

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

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Practical Course work

MCH-203L	ORGANIC CHEMISTRY PRACTICAL - II	Practical (Marks)		Total Credits (Marks)
		I.A (25)	U.E (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 succinicacid 2.2 Diethyl phthalate from phthalicanhydride 2.3 Acetophenone tooxime 2.4 Anthrone fromAnthracene 2.5 Fries rearrangement: Phenylacetate 2.6 Mannichreaction 2.7 Cannizzaroreaction 2.8 Aldolcondensation 2.9 Diazotizationcouplings 2.10 Phenolphthalein from phthalicanhydride.
3.	UV, IR spectra and melting points of simple compounds.

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.

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MCH-204 Paper IX	SURFACE CHEMISTRY	Theory(Marks)		Total Credits (Marks)
		U.E (75)	I.A(25)	03 (100)

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

Unit I: Adsorption **12 L**

Surface tension, Capillary action, Pressure difference across curved surface (Laplace equation), Vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET adsorption isotherm, 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 Catalysis **08 L**

General characteristics of catalytic reactions, Acid-base catalysis, Enzyme catalysis, Mechanism and kinetics of enzyme-catalysed reactions, Michaelis-Menten equation, Heterogeneous catalysis, Surface reactions, Autocatalysis and Oscillatory reactions

Unit III: Micelles **12 L**

Surface active agents, Classification of Surface active agents, Co-surfactants, Micellization, Micro-emulsions, Aggregate structures of surfactants, Critical Micellar Concentration, Surfactant packing parameter, 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 IV Macromolecules **12 L**

Classification and Chain configuration of macromolecules, Isotactic polymers, Atactic polymers, Syndiotactic polymers, Graft polymers, Electrically conducting polymers, Polymerizations reactions, Kinetics of polymerization, Mechanism of polymerization. Theory of Molecular masses of polymers and their physical determinations by Osmometry, Viscometry and Light scattering methods, Sedimentation, Calculation of average dimensions of various chain structures

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.

Suggested Reading :

1. Principals of Nanoscience and Nanotechnology, M. A. Shah and Tokeer Ahmad, Narosa Publications,2010.
2. Introduction to Colloid and Surface Chemistry 2nd Ed., D. J. Shaw, Butterworths,1970
3. Principles of Physical Chemistry, Puri, Sharma, Pathania, Shoban Lal Nagin Chand & Co., EducationalPublishers.
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

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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 ΔGmix 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

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MCH-205 Paper: X	GROUP THEORY AND SPECTROSCOPY	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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**

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 and Paramagnetic Resonance Spectroscopy : 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. **Electron Spectroscopy:** Introduction-representation of the spectrum- hyperfine splitting in some simple system. Hyperfme, splitting in various structures (methyl radical and bis (Salicylaldimine) Copper(II)). Factors affecting the magnitude of 'g' values. Zerofield Splitting and Kramers,degeneracy **10 L**

Unit IV: Mass Spectroscopy: Principle of mass spectroscopy (instrument, operation and representation of spectra), mass spectrometer, interpretation of mass spectra, fragmentation pattern, mode of fragmentation, nitrogen rule, effect of isotopes, signals of doubly charged ion,applications viz; identification of substances, determination of molecular weight and molecular formula. **15 L**

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, Ellis Harwood.

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, andIBH-Oxford.
3. Fundamentals of Molecular Spectroscopy, Fourth Edition, C.N. Banwell and E.M. McCash,Tata McGraw-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.

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MCH-206 Paper: XI	COMPUTATIONAL METHODS IN CHEMISTRY	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	04 (100)

Objective: The skill paper deals with basics of C programming and its applications in Chemistry. It specifically deals with Concepts used in Modern Computational Chemistry and is useful for students of all disciplines

Unit I: 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). **12 L**

Unit II: Applications to Chemistry:: Titration curves and end-point location; ii) pH of a weak acid; iii) Schrodinger equation in 1D; iv) Kinetics of Oscillatory reactions, v) Calculation of Huckel Molecular orbitals of conjugated molecules (Linear, Cyclic, effect of Hetero atom, N, O, Cl, Br); vi) Application of eigen values to Fast Reaction kinetics; vii) normal coordinate analysis for finding normal modes of vibrations of simple molecules **10 L**

Unit III: ***Numerical Methods****:* Solution of quadratic equation by formula, Numerical methods for the roots of polynomial equations, numerical differentiation, integration (Trapezoidal rule, Simpson's rule) and Introduction to Monte Carlo methods, Monte Carlo Integration. solution of ODE, matrix inversion and diagonalization - the jacobi transformation for the diagonalization of a symmetric matrix **12 L**

Unit-IV Introductory Quantum Chemistry Postulates of quantum mechanics. Linear and Hermitian operators. Commutation of operators and Uncertainty Principle. *Some exactly soluble problems:* Particle in a box and ring. Concept of degeneracy and Jahn-Teller distortion. Simple harmonic oscillator problem and its solution using series solution or factorization method. Calculation of various average values using ladder operators and recursion relations of Hermite polynomials. Angular momentum operators, Commutative laws, need of polar coordinates, transformation of Cartesian coordinate into polar coordinate, angular momentum of one particle system. Eigenvalues and eigenfunctions. Ladder operators. Rigid rotator and hydrogen atom: Complete solution. Radial distributions. **14 L**

Essential Reading:

1. Free C Compilers for Windows are availableat:
   (i) http://www.cprogramming.com/code_blocks/ , Instructions for setting up C compiler is given on thisurl.
   (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.
2. Hinchliffe, A. *Modelling Molecular Structures* 2nd Ed., John Wiley & Sons(2003).
3. Press, W. H., Tenkolsky, S. A., Vetterling, W. T. & Flannery, B. P. *Numerical Recipes in Fortran/C* 2nd Ed., Cambridge University Press(1996).
4. Yashavant P. Kanetkar, *Let Us C* 5th Ed.
5. Raman, K.V., Computers in Chemistry, Tata McGraw Hill Education Private Limited,2011.

Suggested Reading:

1. Jurs, Peter C., Isenhour, Thomas L. and Wilkins, Charles L. *BASIC Programming for Chemists: An Introduction*, Wiley-Blackwell(1987).
2. Balagurusamy, E. *Numerical Methods*, Tata McGraw Hill(2000).

M.Sc. CHEMISTRY
SEMESTER - III

MCH-301 Paper no: XII(i)	NMR SPECTROSCOPY AND LANTHANIDE SHIFT REAGENTS	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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.).

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MCH-302 Paper No : XIII(i)	INORGANIC REACTION MECHANISM	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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).

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MCH-303 Paper No : XIV(i)	ORGANOMETALLIC CHEMISTRY - I	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	03 (100)

Objective: Introduction to fundamental concepts in Organometallic chemistry

12 L

Unit I: Organometallics- Main Group and Transition Elements

Introduction, general classification- main group,transitionand inner transition elements organometallics, Nomenclature of organometallic compounds, Synthesis oforganometallic compounds- viz: direct synthesis, redistribution method, metal exchange, ligand exchange, addition reaction, cyclization, sigma-pi -rearrangements and substitutionmethods...

Unit II: Metal Carbonyls, Nitrosyls, Dinitroge and Oxygen Complexes. **12 L**

Metal carbonyls, structure and bonding, Vibrational spectra of metal carbonyls for bonding and structural elucidation. Important reactions of metal carbonyls; preparation; bonding, structure and important reactions of transition metal nitrosyls; dinitrogen and oxygen complexes; Tertiaryphosphine as ligand.

14 L

Unit III: Metal-Alkyls, Aryls, Allyls and Cyclopentadienyl Complexes

Structure and bonding in metal alkyls, allyls and cyclopentadienyl,aryl derivatives with special reference to Ziese's salt and metalocenes.Reactions of cyclopentadienyl, arene pi-complexes – alkylation, acylation ,arylation, Sulphonation ,formylation , Condensation reactions, Addition reactions, Oxidation reactions

Unit IV: Isomerism in Organometallic **12 L**

Isomerism in organometallic complexes – Geometrical, Structural, Conformationals and Optical isomerism, Structure elucidation of metal pi-complexes – special reference to Zieses Salt andmetalocenes.

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 and R.G.Finke, University ScienceBook.
3. The Organometallic Chemistry of the transition metals, R.H.Crabtree, JohnWiley,(1988).

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MCH-304 Paper No : XV(i)	BIO-INORGANIC CHEMISTRY–I	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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 organisms, transport and storage of Inorganic elements, Dose response of an element, biological function of inorganicelements, beneficial and toxic elements, essential and tracemetals

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, ironbiominerals.

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 ScienceBooks.
2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J. S. Valentine,University Science 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).

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Practical Course Work

INORGANIC CHEMISTRY PRACTICAL -III	Theory (Marks)		Total Credits (Marks)
	U.E (75)	I.A (25)	04 (100)

S.No **EXPERIMENT**

1. **Preparations**
   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 oxalatehydrate.
   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. **Spectrophotometric Determination**
   2.1 Mn/Cr/V in steelsample
   2.2 Mo/W/V/U/ by extractive spectrophotometricmethod
   2.3 $F^-/NO_2^-/PO_4^{3-}$
   2.4 Iron-phenanthroline complex: Jobs method of continousvariations.
   2.5 Zr-Alizarin Red-S complex: Mole ratiomethod.
   2.6 Cu-Ethylenediamine complex:Slope-RatioMethod

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

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).

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MCH-305 Paper No : XII(ii)	CONVENTIONAL CERAMICS	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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, electronic configuration of atoms, bonding, Polymorphic forms and transformations, Physical , thermal, electrical, magnetic properties of ceramics

12 L

Unit II: Ceramic Insulators

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 insulating films, thin and thick films- composition and application, sealing glass composition and applications. Procelain: triaxial porcelain- composition and application, non feldspathic porcelains compositions and applications

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 performanceparameters

14 L

Unit IV: Aerogel

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,NewYork

Suggested Reading:

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

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SEMESTER - III

MCH-306 Paper No : XIII(ii)	BASIC CONCEPTS OF CRYSTALLOGRAPHY & CRYSTAL STRUCTURES	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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).

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MCH-307 Paper No : XIV(ii)	POLYMER CHEMISTRY AND TECHNOLOGY	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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 1 **12 L**

Polymers of Commercial Importance, Mass Polymerization: Solution, Emulsion and Suspension Polymerizations, Ziegler Natta Coordination Polymerization, Methathesis 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 JMGCowie
2. Principles of Polymerization by GeorgeOdian

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MCH-308 Paper No : XV(ii)	CHEMISTRY OF ADVANCED MATERIALS	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	03 (100)

Objective: Introduction to types 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, WileyEastern.
2. Handbook of Liquid Crystals, Kelkar and Hatz
3. Thermotropic Liquid Crystals, Ed., G. W. Groy, Chemie Verlog, JohnWiley.

Suggested Reading

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

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ELEMENTS OF MATERIALS CHEMISTRY PRACTICAL-I	Practical (Marks)		Total Credits (Marks)
	UE (75)	IA (25)	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 theTeacher–in-Charge
3. Crystal and crystal growing by Alam Holden and PhylisSinger
4. A laboratory manual of Polymers by S.M.Ashraf, Sharif Ahmad and UfanaRia
5. Practical course in Polymer Chemistry byPinner
6. Experiments in Polymer Chemistry byBillmeyer

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MCH-309 Paper No : XII(iii)	METHODS IN ORGANIC SYNTHESIS	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	03 (100)

Objective: The unit comprises of methods adopted for Organic Synthesis

Unit I Formation of C-C single bonds **8 L**

Generation of thermodynamic and kinetic enolates Alkylation of enolates and enamines, Silyl enol ethers, Conjugate addition reactions of enolates and enamines, Michael addition, Aldolreactions,Evansaldolreaction,Mukaiyamaaldolreactionandstereoselectivealdol reactions. Baylis-Hillman, Robinson annulation, and Prins cyclization reaction**.**

12 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.

Unit III: Oxidations **08 L**

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.

14 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**.**

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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 University Press(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 ChemistryAddison-Wesley Educational Publishers, Inc.(1981).

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MCH-310 Paper No : XIII(iii)	ADVANCED TOOLS IN ORGANIC SYNTHESIS	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	03 (100)

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

Unit I Strategic applications of named reactions: **12 L**

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 indolizationreactions.

Unit II: Rearrangements

General mechanistic considerations-nature of migration, migratory aptitude,memory effects. 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 **08 L**

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, Mukaiyama and Mitsnobu etc.

Unit IV: Organometallics in organic synthesis: **14L**

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

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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. Freemanand Company,2006

Suggested Reading:

1. Organometallic and bioinorganic chemistry by AjayKumar.
2. Organometallic·Chemistry- R.C. Mehrotra & A. Singh, Wiley EasternLtd.(2000)

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MCH-311 Paper No : XIV(iii)	REAGENTS AND ORGANIC SYNTHESIS	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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 andHall).
3. Protective groups in Organic Synthesis Theodora W. Greene & Peter G.M.Wuts.

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MCH-312 Paper No : XV(iii)	CHEISTRY OF HETEROCYCLIC COMPOUNDS	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	03 (100)

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

Unit I Three and four membered heterocycles: **12 L**
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.

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

14 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**.**

Essential Reading:

1. T.L. Gilchrist, Heterocyclic Chemistry, 3rd Edition (1997) Addison-WesleyLongmanLtd., 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, OxfordUniversity
7. Bioinorganic Chemistry- A Short Course; R. M. Roat- Malone; WileyInterscience;2003.
8. Organometallics and bioinorganic chemistry by AjayKumar.

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Suggested Reading:

1. Inorganic chemistry by D.F Shriver and P.W.Atkins.).
2. R.K. Bansal, Heterocyclic Chemistry: Syntheses, Reactions andMechanisms,
3. 3rd Edition (1999), New Age International, Publisher, NewDelhi.
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 andHall).
6. Protective groups in Organic Synthesis Theodora W. Greene & PeterG.M.Wuts.

Practical Couse Work

ORGANIC CHEMISTRY PRACTICAL-I	Practical (Marks)		Total Credits (Marks)
	UE (75)	IA (25)	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 fromtomatoes.
3.	Preparations, isolation and characterizations: (one/two/three-stage). 3.1 Diels-Alder reaction of anthracene with maleicanhydride 3.2 Deils-alder reaction between furan and maleicacid 3.3 Synthesis of indole from cylohexanone andphenylhydrazine. 3.4 Para- aminoazobenzene fromaniline 3.5 Benzophenone→Benzophenone oxime→Benzanilide(Beckmannrearrangement) 3.6 Anthrone from phthalicanhydride 3.7 Benzoin → Benzil → BenzilicAcid. 3.8 Nitrobenzene →m-dinitrobenzene → m-nitroaniline →m-nitrophenol. 3.9 Pthalic anhydride → phthalimide → anthranilicacid. 3.10 Eosin from phthalicanhydride 3.11 Glucazone fromglucose 3.12 Methylene blue from dimethylaniline

Reference Books

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

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MCH-313 Paper No : XII(iv)	NUCLEAR AND ANALYTICAL CHEMISTRY	Theory(Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	03 (100)

Objective: The unit deals with the basic Concepts of Nuclear Chemistry and Analytical Chemistry

Unit I Natural radioactivity **10 L**

Half-life, mean life. Units of radioactivity, the natural radioactive series, secular and transient equilibrium. Standard α, β, γ and neutron laboratory sources. Nuclear sizes, binding energy per nucleon, nuclear saturation, liquid drop model leading to Weizsacker formula. Regions of fission and fusion. Magic numbers, shell model, ground state nuclear spins. Qualitative idea of collective models. Nuclear scattering and reactions, cross-sections, units, phase shifts, Resonance, Breit-Wigner formula. Qualitative idea of Bohr's picture of a nuclear reaction.
Qualitative idea of the nucleon-nucleon and the complex nucleon-nucleon potential (the optical model).

Unit II: Artificial radioactivity **12 L**

Radioactive isotopes of the elements. The Szilard-Chalmers process. Preparation of suitable compounds containing ^{35}S and ^{131}I. Slow neutron absorption in nuclei. Discovery of induced fission its important features. Broad idea of Breeder reactors. Broad sketch of a fusion reactor. Metallurgy of U and Th. Enrichment of Uranium, separation of heavy water from ordinary water. Production of the Trans-Uranic elements. Detailed study of Pu.

Unit III: Electroanlytical Methods **12 L**

Polarography – Theory, diffusion current, identification of cations, half – wave potential, its significance, voltametry and amperometry. Significance and applications of Polarography.

Unit IV: Thermal Methods **11 L**

Thermogravimetric analysis (TGA), principle of TGA, applications of TGA in qualitative and quantitative analysis of inorganic, organic and polymer material. Principles and applications of Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC) and Thermometric Titrations.

Essential Reading

1. G. Friedlander, J. W. Kennedy and J. M. Miller, Nuclear and Radiochemistry, John Wiley (1981)
2. G. Choppin, J. O. Liljenzin and J. Rydberg, Radiochemistry and nuclear chemistry,Butterworth (1996)
3. Skoog, Douglas A., F. James Holler and Timothy Nieman, Principles of Instrumental Analysis. Fifth Edition. New York. 1998.

Suggested Reading

1. J. Arnikar, Essentials of Nuclear Chemistry, Wiley Eastern Ltd. (1995).
2. B. K. Sharma, Nuclear and Radiation Chemistry, Krishna Publication.
3. H.H.Willard, L.L. Merrit Jr., J.A. Dean, F.A.Settle Jr., Instrumental Method of Analysis, Wadsworth Publishing company, USA, 1986.
4. M.E. Brown, Introduction to Thermal Analysis, Kluwer Academic Publisher, London, 2001.
5. G.W. Ewing, Analytical Instrumentation Handbook, Marcel Dekker Inc, New York, 1990.
6. W.W. Wandlandt , Thermal Analysis, Wiley , New York , 1986.
7. A.Blazek, Thermal Analysis, Van Nostrand Reinhold, London, 1972.

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SEMESTER - III

MCH-314 Paper No: XIII(iv)	ADVANCE SOLID STATE CHEMISTRY	Theory(Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	03 (100)

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

Unit I Concepts of Solids **12 L**

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 $I4_1$.

Unit II: Crystal Defects and Non-Stoichiometry in Solids **10 L**

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.

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 **08 L**

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

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, OxfordScience

Suggested Reading

1. New Directions in Solid State Chemistry, C. N. R. Rao and J. Gopalakrishnan,Cambridge University Press.
2. Principals of Nanoscience and Nanotechnology, M. A. Shah and Tokeer Ahmad,Narosa Publications,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

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SEMESTER - III

MCH-315 Paper No : XIV(iv)	CHEMICAL KINETICS	Theory(Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	03 (100)

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

Unit I: Statistical Theories of Kinetics **15 L**

Activated Complex Theory, Potential energy surfaces- attractive and repulsive forces. Rice-Rammsperger and Kassel (RRK) modeland Marcus refinement of RRK model (RKKM) for the calculation of rate constants of simple unimolecular (isomerization) reactions.

Unit II: Complex Reactions **12 L**

Chain reactions and 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 inhibiton- reversibility and products inhibiton.

Unit III: Reactions Dynamics

11 L

Molecular beams, principle of crossed-molecular beams. Molecular encounters and principle parameters, e.g. Impact parameter, Collision cross-section, Reaction cross-section and relation between reaction cross-section and reaction rate (single velocity). Dependence of collisional cross-section on translational energy.

Probing the transition state, Dynamics of barrier-less chemical kinetics in solution, dynamics of unimolecular reactions.

Unit IV: Fast Reactions **12 L**

Luminescence and energy transfer processes, study of kinetics by stopped-flow technique, relaxation method, flash photolysis and magnetic resonance method. Kinetics of solid-state reactions.

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).

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 Kinetic Methods: Principles of Relaxation Techniques and Applications by C.Kalidas, New Age International (P) limited, Publishers,1996
5. Chemical Kinetics and Dynamics, J.I. Steinfeld, J.S. Francisco and W.L. Hase, 2ndEdition, Prentice Hall International, Inc.,1999.
6. Chemical Kinetics: From Molecular Structure to Chemical Reactivity, by L. Arnaut,Sebastiao Formosinho, Hugh Burrows, Elsevier,2007.

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MCH-316 Paper No : XV(iv)	QUANTUM CHEMISTRY	Theory(Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	03 (100)

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

Unit I Some Exactly Solvable Problems **15 L**

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).

Unit II: Approximate Methods **11 L**

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

Unit III: Angular Momentum, Spin and Electronic Structure **12 L**

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.

Unit IV: Molecular Orbital Theory **10 L**

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).

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.

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SEMESTER - III

Practical Course Work

PHYSICAL CHEMISTRY PRACTICAL-III	Practical (Marks)		Total Credits (Marks)
	UE (75)	IA (25)	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-linemethod (b) double alkalimethod
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 reversetitration (b) HCl versusNH_4OH (c) Sodium oxalate againstHCl.
7.	. Determine the rate constant of saponification of ethyl acetate at different temperatures and calculate the energy of activation of the reacton 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.

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14. Titrate potentiometrically solutions of
(a) KCl/ KBr/KI;
(b) mixture of KCl + KBr + KI and determine the composition of each component in themixture.

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.

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)

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MCH-317 Paper No : XVI	CHEMISTRY OF SYNTHETIC AND NATURAL MATERIALS-I	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	04 (100)

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

Unit I Super conductors: Superconducting state; heat capacity; coherence length, elastic constants, microwave absorption pairing and multi-gap structure in high Tc materials. Applications of high Tc materials. Preparation and characterization of 1-2-3 and 2-1-4 materials. Normal state properties, anisotropy, temperature Dependence of electrical resistance, and optical modes. **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 of analysis, 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. **15L**

Unit-IV Metal Complex sensitizers **12L**

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

Essential Reading

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

Suggested Reading

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

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MCH-318 Paper No : XVII	ENVIRONMENTAL AND GREEN CHEMISTRY	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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 **12 L**

Synthesis and modification of inorganic solid**s:** Conventional heat and beat methods, Co-precipitation method, Sol-gel methods, Hydrothermal method, Ion-exchange and Intercalation methods. Inorganic solids of technological importance**:** Solid electrolytes – Cationic, anionic, mixed Inorganic pigments – coloured solids, white and black pigments. Molecular material and fullerides, molecular materials and chemistry – one-dimensional metals, molecular magnets, inorganic liquidcrystals

Unit III: Handling of Chemicals

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation. Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric – safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals **10 L**

Unit IV: Green Chemistry **15 L**

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. 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., NewDelhi.
4. 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

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SEMESTER - IV

MCH-401 Paper No : XVIII (i)	CHEMICAL APPLICATIONS OF GROUP THEORY	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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 (exampleSF_4).

Unit II: Symmetry Aspects of Hybrid Orbitals **12 L**

Transformations propertiesof atomic orbitals. Hybrid orbitals for sigma bonds in trigonal planar (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.

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.

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MCH-402 Paper No : XIX (i)	STEREOCHEMISTRY AND METAL ION CATALYSIS	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	03 (100)

Objective: Introduction to Advance concepts in Stereochemistry and Metal ion catalysis **12 L**

Unit I: Stereochemical Changes in Octahedral Complexes-I

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.

14 L

Unit III: Photochemical Reactions

Introduction, types of excitation, fate of excited molecules, quantum yield, types of photochemical reactions

Unit IV: Metal Ion Catalysis **12 L**

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

Essential Reading

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

Suggested Reading:

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

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MCH-403 Paper No : XX (i)	ORGANOMETALLIC CHEMISTRY-II	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	03 (100)

Objective: Introduction to Advance concepts in Organometallic chemistry

12 L

Unit I: Fluxionality and Dynamic Equilibria

Fluxionality and dynamic equilibria, Fluxionality in tricarbonyl (Diene) Iron Complexes, Fluxionality in pi-Olefin complexes, Pi-allyl complexes, Tricarbonyl cyclooctatetraene (COT) metal complexes

Unit II: Distinctive organometallic Reactions

12 L

Distinctive organometallic Reactions - Nucleophilic and Electrophilic attack of co-ordinated ligands and elimination reactions, Oxidative – Addition reactions, Insertion reaction – at M-C bond & M-H bond, Transmetallation reaction and Cyclization reaction, , Ring Expansion reaction, Condensation reaction , Sigma-pi rearrangement reaction , Ligand & Metal exchange reactions..

14 L

Unit III: Compounds of Transition Metal-Carbon Multiple Bonds

Alkylidenes, alkylidynes, low valent carbenes and carbynes-synthesis, nature of bond, structure characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis.

Unit IV: Homogeneous Catalysis **12 L**

Catalytic applications of organometallic complexes - Alkene hydrogenation, Synthesis gas (H_2/CO), Hydroformylation, Mosanto-acetic acid process, Wacker- Schmidt process and Ziegler-Natta catalysis. Bioorganometallic chemistry and surface organometallic chemistry..

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 | 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. Comphrensive coordination chemistry Eds.: G. Wilkinson, R.D.Gillards and J.A. McCleverty, Pergamon

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MCH-404 Paper No : XXI (i)	BIO-INORGANIC CHEMISTRY–II	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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, hemotherine

Unit II: Metalloenzyme **12 L**

Principle involved and role of various metals viz. Zn, Fe, Cu and Co; carboxy peptidase, carbonic anhydrase, Alcohol dehydrogenase, Zinc Fingures, 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, cytochrpm P-450, oxygen transfer long distance electron transfer

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

Medicinal and therapic; metal deficiency and disease, toxic effect of metals, metals usedfor diagnosis and chemotherapy, gold compound as Anti-Rheumatic agent. Nitrogen cycle; biological nitrogen fixation, metalloenzyme in biological nitrogen cycle, molybdenum nitrogenase, other nitrogenasemodel

Essential Reading

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

Suggested Reading:

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

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MCH-405 Paper No : XVIII (ii)	TECHNICAL CERAMICS	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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 donars, 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

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. **14 L**

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) MarcelDeller, 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 CHARACTERIZATION OF CRYSTAL STRUCTURES	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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 printing and 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 andanions, 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. AllcockWiley.
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 RobertSnyder.

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

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SEMESTER - IV

MCH-407 Paper No : XX (ii)	POLYMER TECHNOLOGY, PROCESSING AND SPECIALITY POLYMERS	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	03 (100)

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

Unit I: Polymer Technology – II **10 L**

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

Unit II: Unit II: Polymer Processing **10 L**

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

Unit III: Biopolymers **14 L**

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

Unit IV: Speciality Polymers **12 L**

Conductive Polymers: Theory of Conduction, Synthesis and Applications ofConductive Polymers, Biodegradable Polymers, Biomaterials, Polymers in Medicine, DrugDelivery Systems, Recycling ofPolymers

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:

3. Polymers: Chemistry and Physics of Modern Materials by JMGCowie
4. Principles of Polymerization by GeorgeOdian

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MCH-408 Paper No : XXI (ii)	PROPERTIES OF MATERIALS	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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 semi conductors, 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

Unit II: Electrical Properties **14 L**

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

Unit III: Magnetic Properties **10 L**

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

Unit IV: Optical Properties **10 L**

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 byEpifanov.
2. Materials Science by Anderson andlever.

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MCH-409 Paper No : XVIII (iii)	MEDICINAL CHEMISTRY AND BIOMOLECULES	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	03 (100)

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

UNIT- I :Drug design **8 L**

Concept of lead compound, lead modification, prodrugs and soft drugs, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductiveeffect,isosterism,bio-isosterism,spatialconsiderations.Occupancy theory, rate theory, induced fit theory. Concepts of drug receptors. Free-Wilson analysis, Hanschanalysis, relationship between Free-Wilson and Hansch analysis.LD-50,ED-50(Mathematicalderivationsofequationsexcluded).

UNITII: 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 **08 L**

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.

Unit IV: Antimicrobial Drugs **14 L**

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**.**

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.

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MCH-410 Paper No : XIX(iii)	ADVANCED METHODS IN ORGANIC SYNTHESIS	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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) **12 L**
: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), enyne 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.

Unit III: C-H Bond Functionalization/Activation: **08 L**
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..

14 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

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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-VerlagBerlin Heidelberg2007.

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.

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MCH-411 Paper No : XX (iii)	CHEMISTRY OF NATURAL PRODUCTS	Theory (Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	03 (100)

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

Unit ITerpenoids: **12 L**

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

Unit II:Alkaloids: **12 L**

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.

Unit III:Steroids:

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

Unit IV: Prostaglandins and Flavonoids: **14 L**

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

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,Naturalproducts chemistry 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.

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MCH-412 Paper No : XXI (iii)	APPLICATIONS OF SPECTROSCOPY	Theory(Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	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:

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. **08 L**

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 OrganicCompounds, 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, PrenticeHall.
6. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGrawHill.
7. Organic Spectroscopy, Second Edition, W. Kemp, ELBS Macmillan, 1987 for RD and CD andESR.

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MCH-413 Paper No : XVIII (iv)	ADVANCED MOLECULAR SPECTROSCOPY	Theory(Marks)		Total Credits (Marks)
		U.E(75)	I.A (25)	04 (100)

Objective: The unit deals with the Physical Aspects of Spectroscopy

Unit I: Introduction to Molecular Spectroscopy **15 L**

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.

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 **10 L**

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.

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 **09 L**

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

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

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MCH-414 Paper No : XIX (iv)	NANO CHEMISTRY	Theory(Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	04 (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.

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MCH-415 Paper No : XX (iv)	ADVANCED PHYSICAL CHEMISTRY	Theory(Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	04 (100)

Objective: The unit deals with the Concepts of Biophysical chemistry

Unit I Fundamentals of Biological Macromolecules: **12 L**

1. Chemical bonds in biological systems; 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: **06 L**

Polypeptide chain geometries and internal rotational angles: Ramachanrdan plots; Molecular mechanics; Stabilizing interactions in biomolecules.

Unit III: Phase Equilibria and Phase Transformations: Multicomponent systems, the lever rule, Thermodynamic treatment of kinetics of internal processes, Transport processes in continuous and discontinuous systems, Onsager's extremum principle, Some necessary conditions of stability, Limit of stability against fluctuations in composition, Chemical capacitance, Applications of molar Gibbs energy diagrams for binary & ternary systems, Allotropic phase boundaries, Partitionless transformation under local equilibrium, Activation energy for a fluctuation, topology of potential phase diagrams in binary and multinary systems, Sections of potential phase diagrams, Molar phase diagrams, Sections of molar phase diagrams, Schreinemakers' rule, Topology of sectioned molar diagrams, Projected and mixed phase diagrams, Direction of phase boundaries, Sharp and gradual phase transformations, transformations in closed systems. **14L**

Unit IV: Thermochemistry **10L**

Concept of heat of reactions; Thermochemical equations; Standard states; Relation between heat of reaction at constant volume (q_v) and heat of reaction at constant pressure (q_p),; Laws of thermochemistry; Various types of heat changes; Born-Haber cycle; Bond energies; Variation of heats of reaction with temperature and variation of heats of reaction with pressure.

Essential Reading

1. C. R. Cantor & Schimmel. Biophysical Chemistry Vols 1-3,, W. H. Freeman (1980).
2. Y. Moroi, Micelle – Theoretical and applied Aspects, Plenum Press, New York, 1992.
3. Mats Hillert, Phase Equilibria, Phase Diagrams and Phase Transformations, 2nd Edition, Cambridge University Press, UK (2008).
4. Thermodynamics, J. Rajaram and J.C. Kuriacose, Educational Publishers.

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Essential Reading

1. J. O. M. Bockris, A. K. N. Reddy and M. Gamboa – Aldeco: Modern Electrochemistry, Vol. 2A, Fundamentals of Electrodics, 2nd Ed. Plenum Press, New York,2000.
2. Y. Moroi, Micelle – Theoretical and applied Aspects, Plenum Press, New York,1992.

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SEMESTER - IV

MCH-416 Paper No : XXI (iv)	ELECTROCHEMISTRY	Theory(Marks)		Total Credits (Marks)
		U.E (75)	I.A (25)	04 (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 capacitance of 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., Plenum Press, 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 (75)	I.A (25)	04 (100)

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

Unit I: Applications of High Tc Materials: **15 L**

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

Unit II: Supramolecular Chemistry **12 L**

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

Unit III: Advance Quantum mechanics **10 L**

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

Unit IV: Excited state of metal Complexes **15 L**

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

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.

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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.