Rev: 04

SYLLABUS

For

2 YEARS MSC IN CHEMISTRY PROGRAMME

(Revised Syllabus Approved by Academic Council)

Unveiling Excellence

Dept. of

Chemistry

JUNE, 2019

UNIVERSITY OF SCIENCE &TECHNOLOGY, MEGHALAYA

Techno City, 9th Mile, Baridua, Ri-Bhoi, Meghalaya, 793101

Syllabus Contents

Programme: Master of Science
Department: Chemistry
School: SOAS

About the Department:

Established in the year 2012, the Department of Chemistry has been providing higher education in chemistry by training students through its ongoing B.Sc., M.Sc. and Ph.D programmes. The academic curriculum of the department has been framed to enable the students to achieve a good understanding of the subject. The Department already has developed a strong association with the leading research institutes of the region to collaborate on research grounds. The research activities are currently centered at environmental chemistry, synthetic methodologies and catalysis.

Academic Focus:

The Department focuses on the areas which reflect the technical know-how of current research and we aim to develop teaching and research in these fields of chemistry. We collaborate with different stake holders and organizations to create new inputs and materials into our teaching and research.

Career Scope:

The curriculum of the department of chemistry, USTM is framed to provide both basic and applied knowledge in the field of chemistry. The employment opportunities for chemical professionals can be divided into five main sectors: industry, academia, government, non-profit, and entrepreneurship.

Programme Details:

The Department of chemistry provides 2 (two) years Master of Science (M.Sc.) program with 2 (two semesters). The program is designed to cater to the need of the students who intend to persue a career within academia, outside the academia and in R&D sector. The program provides students with the opportunity to develop knowledge, understanding, knowledge and expertise in the field.

Eligibility Criteria: B.Sc. 50 % marks.

Programme Objectives (PO)

The programme provides scienctific skills and knowledge essential for success in the field. The Programme aims to train proper laboratory techniques and safety protocols so as to enable the students persue career in higher education and in R&D sector. It also equips students with effective scientific skills and commitment towards ethical and social responsibilities.

Programme Specific Outcomes (PSO)

Programme Name: Master of Science

Programme Code: M.Sc.

PSO1: Sound knowledge about the fundamentals of theories concerning behind formation of new substances.

PSO2: To appropriately apply techniques for the qualitative and quantitative analysis of chemicals in laboratories and industries.

PSO3: To develop analytical skills and problem solving skills requiring application of chemical principles.

PSO4: To become familiar with the different branches of chemistry like analytical, organic, inorganic, physical, environmental, polymer, biochemistry etc.

PSO5: To Acquire the ability to undertake independent research**.**

PSO6: To understand the different issues of environmental concern and sustainable solution.

Programme Structure:

The B.Sc. programme is a three year program divided into six semesters. The programme is of 140 credits and for the award of degree a student will be required to complete the credits as per the University norm.

SEMESTER-I

Course Code	Title	Credit	Nature of course (T/P)	Marks Allotted		
				Internal	End Semester	Total
MSC 101	Inorganic Chemistry I **(CC-1)**	4	T	30	70	100
MSC 102	Organic Chemistry I **(CC-2)**	4	T	30	70	100
MSC 103	Physical Chemistry I **(CC-3)**	4	T	30	70	100
MSC 104	Quantum Chemistry and Molecular Spectroscopy I **(CC-4)**	4	T	30	70	100
MSC 105	Organic Chemistry Practical **(CC-5)**	4	P	30	70	100
Total		**20**		**150**	**350**	**500**

SEMESTER-II

Course Code	Title	Credit	Nature of course (T/P)	Marks Allotted		
				Internal	End Semester	Total
MSC 201	Inorganic Chemistry II **(CC-5)**	4	T	30	70	100
MSC 202	Organic Chemistry II **(CC-6)**	4	T	30	70	100
MSC 203	Physical Chemistry II **(CC-7)**	4	T	30	70	100
MSC 204	Quantum Chemistry and Molecular Spectroscopy II **(CC-5)**	4	T	30	70	100
MSC 205	Inorganic Chemistry Practical **(CC-6)**	4	P	30	70	100
Total		**20**		**150**	**350**	**500**

SEMESTER-III

Course Code	Title	Credit	Nature of course (T/P)	Marks Allotted		
				Internal	End Semester	Total
MSC 301	Inorganic Chemistry III **(CC-7)**	4	T	30	70	100
MSC 302	Organic Chemistry III **(CC-8)**	4	T	30	70	100
MSC 303	Physical Chemistry III **(CC-9)**	4	T	30	70	100
MSC 304	Applications of Spectroscopy **(CC-10)**	4	T	30	70	100
MSC 305	Physical Chemistry Practical **(CC-11)**	4	P	30	70	100
MSC 306 A / 306 B	Environmental pollution and management / Green Chemistry **(GE-1)**	4	T	30	70	100
Total		**24**		**180**	**420**	**600**

SEMESTER-IV

Course Code	Title	Credit	Nature of course (T/P)	Marks Allotted		
				Internal	End Semester	Total
MSC-401 A / MSC-401 B / MSC-401 C)	Natural Product Chemistry / Bioinorganic And Inorganic Photochemistry / Chemical Dynamics And Electrochemistry **(DSE-1)**	4	T	30	70	100
MSC-402 A / MSC-402 B / MSC-402 C	Medicinal Chemistry / Materials Chemistry and Nanomaterials / Solid State And Polymer Chemistry **(DSE-2)**	4	T	30	70	100
MSC-403	Physical Methods of Analysis **(CC-12)**	4	T	30	70	100
MSC-404	Project work **(CC-13)**	8	P	60	140	200
MSC 406	Trends in Polymer Science and Technology / Testing of Pharmaceutical Drugs **(SEC-3)**	Non Credit Mandatory				
Total		**20**		**150**	**350**	**500**

Semester	Core Courses ()	Ability Enhancement Compulsory Courses [AECC] ()	Skill Enhancement Course [SEC] ()	Discipline Specific Elective [DSE] ()	Generic Elective [GE] ()
I	Inorganic Chemistry I				
	Organic Chemistry I				
	Physical Chemistry I				
	Quantum Chemistry and Molecular Spectroscopy I				
	Organic Chemistry Practical				
II	Inorganic Chemistry II				
	Organic Chemistry II				
	Physical Chemistry II				
	Quantum Chemistry and Molecular Spectroscopy II				
	Inorganic Chemistry Practical				
III	Inorganic Chemistry III				Environmental pollution and management / Green Chemistry (GE)
	Organic Chemistry III				
	Physical Chemistry III				
	Applications of Spectroscopy				
	Physical Chemistry Practical				
IV	Physical Methods of Analysis			Natural Product Chemistry / Bioinorganic And Inorganic Photochemistry / Chemical Dynamics And Electrochemistry **(DSE-1)**	Everyday Chemistry/ Biological Chemistry **GE-1)**
	Project work			Medicinal Chemistry / Materials Chemistry and Nanomaterials / Solid State And Polymer Chemistry **(DSE-2)**	

MSC 101: INORGANIC CHEMISTRY I **Marks: 30+70=100**
Total Credits: 4

***Objective*: Introduction to metal-ligand bonding, electronic spectra and knowledge of basic chemistry of compounds of non-transition elements.**

***Course Outcome*: Interpretation of electronic spectra and understanding of chemistry of compounds of non-transition elements.**

CO1: To give the knowledge of molecular structure and bonding of different molecules.

CO2: To give the knowledge of metal-ligand bonding in d-block element.

CO3: To give the knowledge of electronic spectra of d-block metal complexes.

CO4: To give the knowledge of non-transition elements.

CO5: To give the knowledge of Metal Clusters.

CONTENTS:

Unit I: Molecular Structure and Bonding.

Molecular Orbital theory-Homo-nuclear molecules (H2 to F_2), Hetero-nuclear molecules (CO, NO) Polyatomic molecules (BF3, B_2H_6, SF_6). Bond Properties- Bond Length, Bond strength, Electronegativity and bond enthalpy.

Unit II: Metal–Ligand Bonding in Transition Metal Complexes

Crystal Field theory, Ligand Field Theory, Jahn-Teller distortions, crystal field stabilization energy, spectrochemical series, thermodynamic aspects of crystal field splitting (variation of ionic radii, lattice-energy, hydration energy), kinetic aspects of crystal field splitting (labile and inert complexes), octahedral vs tetrahedral coordination. Qualitative MO treatment: the electronic structure of the ML_6 (octahedral) and ML_4 (tetrahedral) complexes on the basis of simple symmetry and overlap principles, energy level diagrams, (for σ- bonding and π-bonding complexes).

Unit III: Electronic Spectra of Transition Metal Complexes

Spectroscopic terms, Racah parameters; d-d transitions in weak and strong field cases, (Octahedral and Tetrahedral complexes) Orgel and Tanabe Sugano diagrams of transition metal complexes (d^1-d^9 states), Charge transfer spectra, Intensity of bands, Laporte and Spin selection rules and relaxation. splitting of f-orbitals in octahedral field.

Unit IV: Chemistry of non–Transition elements and Clusters

General discussion on the properties of the non-transition elements, special features of individual elements, synthesis, properties and structure of halides and oxides of non–transition elements; Polymorphism in carbon, fullerenes, phosphorus and sulphur; Synthesis, structure and properties of boranes, carboranes, metallocarboranes, silicates, carbides, phosphazenes.

Suggested Readings

MSC 101 INORGANIC CHEMISTRY I

Text Books / Reference Books:

1. J. E. Huheey, E. A. Keiter, R. L. Keiter& O. K. Medhi. Inorganic Chemistry: Principles of Structure and

Reactivity, Pearson Education (2006).

2. F. A. Cotton, G. Wilkinson, C. A. Murillo & M. Bochmann. Advanced Inorganic

Chemistry (6th edition), John Wiley (1999).

3. M. Weller,T. Overton, J. Rourke, & F. Armstrong, Inorganic Chemistry, Oxford University Press , 6^{th} edition.

4. J. D. Lee, Concise Inorganic Chemistry, Elbs, Chapman and Hall, 2006.

5.G. L.Meissler and D. A. Tarr; Inorganic Chemistry, 3^{rd}. Edition, Pearson.

6. B. Douglas, D. McDaniel and J. Alexander. Concepts and Models of Inorganic Chemistry

(3rd edn.), John Wiley & Sons (1994).

7. B. R. Puri, L. R. Sharma and K. C. Kalia; Principles of Inorganic Chemistry. Vishal Pub. 2016.

MSC 102 ORGANIC CHEMISTRY I **Marks: 30+70=100**
Total Credits: 4

Objective: **Objective of the course is to provide the concepts of reaction mechanism, reaction intermediates and stereochemistry.**

Course Outcome: **Students will be able to understand and solve the problems of organic reaction through mechanism, reaction intermediates and stereochemistry.**

CO1: To give the knowledge of organic reactive intermediates and their role in organic reactions.

CO2: To give the knowledge of different reaction pathways for variation organic reactions.

CO3: To give the knowledge of molecular orientation in space and its identification.

CO4: To give the knowledge of symmetric synthesis and different rulings on identification of major products.

CO5: To give the knowledge of Aromaticity in organic molecules

CONTENTS

UNIT-I: Structure and Reactivity
A. Strength of acids and bases. Introduction to aromaticity in Benzenoid and non–Benzenoid compounds, Azulenes, Tropolenes, (4n+2) Huckel rule and it's applications, Frost diagram. Effect of structure on reactivity. The Hammett equation and linear free energy relationship, modifications of Hammett equation.
B. Generation, structure, stability and reactivity of carbocations, carbanions, ylides, free redicals, carbenes, ketenes, nitrenes, and benzynes.

UNIT-II: Reaction Mechanism I
A. Nucleophiles-definition, types-anionic, neutral, hard, soft, ambident. Reactivity effect of substrate structure, effect of attacking nucleophiles, leaving groups and reaction medium. Neighbouring group participation.
B. Nucleophilic substitution reactions– SN^1, SN^2 and SN^i mechanism and stereochemistry. Aromatic Nucleophilic Substitution: The SNAr, S_N1, benzyne and SR_N1 mechanisms. Nucleophilic substitutions at an allylic, aliphatic trigonal and vinylic carbons. Isotope labeling and kinetic isotope effects.

UNIT-III: Reaction Mechanism II
A. Elimination reactions: E^1, E^2, E^{1CB}; mechanism, orientation and stereochemistry of Elimination, Umpolung, Protection-deprotection chemistry of selected functional groups such as aldehydes, ketone and –OH, $–NH_2$.

B. Aromatic Electrophilic Substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring system. Quantitative treatment of reactivity in substrates and electrophiles.

UNIT-IV: Stereochemistry

A. Fischer, Newman, Sawhorse and flying wedge projections and their interconversions. Conformational analysis of aliphatic organic molecules, cycloalkanes and decalins. Effect of conformation on reactivity in acyclic and cyclohexane systems. Molecules with more than one asymmetric centre e.g. erythro and threo compounds, D, L notations. R, S notations of biphenyles and allenes. Concepts of stereogenic centres – chirotopic and achirotopic centres, homotopic and heterotopic ligands and faces, optical purity and enantiomeric excess.

B. Chirality due to helical shape, a brief Study of dissymmetry of allenes, biphenyls and spiro compounds. Stereo specific and stereo selective reactions. Asymmetric synthesis, enantioselective and diastereoselective synthesis. Cram's and Prelog's rule, Cram model, Felkin-Ahn model.

Suggested Readings

MSC 102 ORGANIC CHEMISTRY I

Text Books/Reference Books:

1. S. H. Pine. *Organic Chemistry* (5th edn.), McGraw-Hill Bool (2012).
2. Organic Chemistry by T.W. Graham Solomons and Craig B. Fryhle (10^{th} Edition), Willy Student Edition (2012)
3. Advanced organic chemistry by J. March, (4th Ed) (2008) published by Wiley
4. A guidebook to mechanism in organic chemistry – Peter Sykes (6th Ed) Orient Longman (2005)
5. Organic Reactions and their mechanisms (3^{rd} revised edition) by P.S. Kalsi, New Age International (P) Ltd (2010)
6. Reaction Mechanism and Reagents in Organic Chemistry -Gurdeep R Chatwal, New Age International (P) Ltd (2010)
7. Organic Chemistry (VI edition) - R.T Morrison, R.N. Boyd. Prentice Hall of India Pvt Ltd, (2009)
8. Organic Chemistry - I.L. Finar, 6th Edition (Low price) Pearson Education, 2009

MSC 103: PHYSICAL CHEMISTRY I **Marks: 30+70=100**

Total Credits = 4

Objective: **Students will be introduced to chemical kinetics, equilibrium and non-equilibrium thermodynamics, polymers and data analysis will also be covered.**

Course Outcome: **to apply the knowledge to understand different chemical reactions and statistical data interpretations.**

CO1: To give the knowledge of kinetics of different reaction and their mechanism.

CO2: To give the knowledge of equilibrium and non-equilibrium thermodynamics.

CO3: To give the knowledge of non-equilibrium thermodynamics.

CO4: To give the knowledge of chemistry of polymerization and its applications.

CO5: To give the knowledge of evaluation of analytical data.

CONTENTS

Unit I: Chemical Kinetics I

Methods of determining rate laws, Steady state approximation and its applications, Mechanism of photochemical (hydrogen-bromine and hydrogen-chlorine), chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde), consecutive and oscillatory reactions (Belousov-Zhabotinski reaction)

Collision theory of reaction rates, collision cross-sections, rate coefficient, steric factor, Straight chain reactions, the hydrogen-oxygen reaction, explosion limit. Theory of absolute reaction rates, activated complex theory, thermodynamic interpretation, comparison of results with Erying and Arrhenius equations. Numerical Problems

Unit II: Equilibrium Thermodynamics and Non-equilibrium thermodynamics

Brief review of thermodynamic functions and laws of thermodynamics. Temperature dependence of thermodynamic functions. Gibbs-Helmholtz equation, partial molar properties: partial molar Gibbs free energy, partial molar volume, partial molar heat content and their significances. General methods of determination of partial molar properties – Gibbs-Duhem and Gibbs-Duhem-Margules equation, excess thermodynamic functions. Third law of thermodynamics, calculation of entropy, Residual entropy.

Non-ideal system: thermodynamics of real gases and gas mixtures, fugacity and its determination, non-ideal solutions, activity and activity coefficient-different scales of activity coefficient, electronic activity coefficients

Thermodynamic criteria of phase equilibrium, Gibbs phase rule and its application to one, two & three component systems - triangular plots-water-acetic acid-chloroform system.

Non-equilibrium thermodynamics: forced flows and entropy of production, coupled flows and phenomenological relations, Onsager reciprocal relations, thermodynamic effects- Seebeck and Peltier and Thomson effect

Unit III: Polymers

Polymer: Functionality and polymerization concept, Number average, weight average, viscosity average, sedimentation average molecular weights. Molecular weight distribution, polydispersity and degree of polymerization, End group Analysis.

Chemistry of Polymerization: Free radical chain polymerization, kinetics of free radical polymerization, Cage effect and chain transfer reactions. Chemistry and kinetics of Condensation polymerization, Coarother's equation. Cationic and anionic polymerization chemistry, kinetics and degree of Polymerization. Copolymerization, types, copolymerization equation, monomer reactivity.

Unit IV: Errors and Evaluation of Analytical Data

Definition of terms, Precision, deviation, mean deviation, standard deviation, accuracy, absolute errors, types of errors determinate, indeterminate and gross, sources of errors and their effect on final result, Methods of reporting analytical data. Statistical evaluation of data. Indeterminate errors, linear least squares methods, correlation coefficient. Significant figures, Problems.

Suggested Readings

MSC 103: PHYSICAL CHEMISTRY I

Text Books/Reference Books:

1. Atkins Physical Chemistry, Peter Atkins & Julio D Paula, Oxford University Press, 2006.
2. Principles of Physical Chemistry by B.R. Puri, L.R. Sharma, Madan S. Pathania, Vishal Publishing Company, 2008.
3. Text book of polymer science: F.W. Billmeyer, (John.Wiley), London, 1994.
4. Polymer science: V.R. Gowariker, N.V. Viswanathan & T. Sreedhar, (Wiley Eastern) New Delhi, 1990.
5. Introduction to Physical polymer science, L.H. Sperling, Wiley Interscience, New York, 1986.
6. Physical Chemistry (Vol. 1 & 2), K.L. Kapoor, Macmillan, 2001.
7. Physical Chemistry (Vol. 1 & 2), Ira N Levine, Macmillan, 2001.

MSC 104: Quantum Chemistry and Molecular Spectroscopy I **Marks: 30+70=100**
Total Credits: 4

Objective: **Introduction to fundamentals of quantum chemistry and molecular spectroscopy**

Course Outcome: **Students will be able to understand the theoretical basis of Quantum chemistry and spectroscopic techniques of rotational, vibrational and Raman spectroscopy.**

CO1: To give the knowledge of principle of quantum mechanics.

CO2: To give the knowledge of applications of quantum mechanics to model systems

CO3: To give the knowledge of molecular spectroscopy related to electromagnetic radiations.

CO4: To give the knowledge of rotational and vibrational spectroscopy.

CO5: To give the knowledge of vibrational spectroscopy.

CONTENTS:

A. Quantum Chemistry

Unit I: Principles of Quantum Mechanics

Review of the basic principles of quantum mechanics: Postulates, Schrödinger equation, normalization and orthogonalization of wave function. Expectation values, Quantum mechanical operators, Hamiltonian operator, Hermitian operators, angular momentum operator.

Unit II: Model Systems

Translational Motion: Free particle and particle in a box (one, two and three dimensional)

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wavefunctions. Vibrational energy of diatomic molecules and zero-point energy. Hermite polynomials, rigid rotor, particle in a ring, quantum mechanical tunneling.

B. Molecular Spectroscopy

Unit III:

Electromagnetic Spectrum: Interaction of electromagnetic radiation with molecular systems. Spectroscopic transitions-adsorption, emission, reflection, polarization and scattering process. Natural line width and broadening - Intensity of spectral transitions, selection rules.

Unit IV

Rotational Spectroscopy: Classification of molecules according to moment of inertia. Rotational energy levels of HCl molecules. Spectra of linear, symmetric top and asymmetric top type molecules. Isotopic effect on pure rotational spectrum. Stark effect, estimation of molecular dipole moment. Spectra of asymmetric top and asymmetric top type molecules.

Unit VI

Vibrational Spectroscopy

Fundamental vibrational frequencies, selection rules and vibrational energy for harmonic and anharmonic oscillators, vibration-rotation spectroscopy, diatomic vibrating rotator, fundamental, overtone and P, Q, R branches, hot bands, group frequencies, normal modes of vibrations.

Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.

Suggested Readings

MSC 104 Quantum Chemistry and Molecular Spectroscopy I

Text Books/Reference Books:

1. Introductory Quantum Chemistry, A. K. Chandra. Tata McGraw Hill, 1994.
2. Quantum Chemistry, I. N. Levine, Prentice Hall India, 2001.
3. Quantum Chemistry, B K Sen
4. Fundamentals of Molecular Spectroscopy by Colin N. Banwell & Elaine M. McCash

(4^{th} Edition) 2009 Published by Tata McGraw-Hill Publishing Company Ltd.

MSC 105: ORGANIC CHEMISTRY PRACTICAL **Marks: 30+70=100**
Total Credits: 4

Objective: Students will be introduced to common laboratory practices, techniques/apparatus for carrying out a synthesis of organic compounds and extraction of natural products

Course Outcome: Students will be able to perform qualitative and quantitative analysis of organic compounds and mixtures, implement multi-step organic synthesis and operate common/sophisticated instruments.

CO1: Practical knowledge of elemental constituents of organic molecules.
CO2: Practical knowledge of identification of various functionalities of organic molecules.
CO3: Practical knowledge of different separation techniques of organic mixtures.
CO4: Practical knowledge of synthetic strategies of organic molecules.
CO5: Practical knowledge of extraction of natural products

CONTENTS:

1. (a) Purification of binary mixtures by Thin Layer Chromatography (TLC) and Column Chromatography (CC).
(b) Purification of tertiary mixtures of amino acids by Paper Chromatography.
2. Quantitative Analysis of solid organic sample
(i) Detection of elements (N, Cl, Br, I, S), solubility test, unsaturation and aromaticity.
(ii) Systematic Analysis to detect the functional groups:
Alcoholic/phenolic OH, carboxylic, aldehyde, ketone, ester, ether, nitro, amido, N-substituted amino, imido groups.
(iii) Preparation of crystalline derivatives/ suitable derivatives to identify the compound.
3. Extraction of Natural products: any one of the following-solasodine, caffeine, nicotine, piperine, carotenoids.
4. Organic preparations: At least eight preparation (involving two or more steps) involving the following representative reactions -

(a) Esterification and saponification
(b) Oxidation (peracid, chromic acid, Mn(VII)
(c) Hydride reduction or hydrogenation
(d) Nucleophilic substitution
(e) Cycloaddition reaction
(f) Grignard reaction
(g) Condensation reaction
(h) Preparation of dyes
(i) Aromatic electrophilic substitution
(j) Heterocyclic synthesis
(k) Pinacol-Pinacolone rearrangement
(l) Benil-Benzilic acid rearragement
(m) Aspirin

Suggested Readings

MSC 105: ORGANIC CHEMISTRY PRACTICAL

Text books/ References Books:

1. R. K. Bansal, Laboratory of organic chemistry (3rd edn), Wiley-Eestern, 1994.
2. R. K. Brewster & W. E. Mcwerdn. Unitized experimental organic chemistry (4th edn), East-West press (1977).
3. A. I. Vogel, Practical organic chemistry (5th edn), Longman Group Ltd. (2009).
4. V K Ahluwalia, R Agarwal. Comprehensive Practical organic chemistry – preparation and quantitative analysis, University Press (2013)
5. O. Fitton & R. K. Smallery, Practicat heterocyclic chemistry.
6. R. L. Shriner & R. C. Fusion, Systematic Identification of organic compounds (5th edn.), John Wiley Sons (1964).

MSC 201: INORGANIC CHEMISTRY II **Marks: 30+70=100**

Total Credits: 4

Objective: **Knowledge of symmetry, structure of solids and chemistry of transition elements**

Course Objective: **Interpretation of application of symmetry to spectra and MOT of bonding, diverse chemistry of transition metal compounds**

CO1: To give the knowledge of symmetry of molecules and its application.

CO2: To give the knowledge of various transition metal complexes and their magnetic properties.

CO3: To give the knowledge of Magnetic properties of transition metal complexes.

CO3: To give the knowledge of oxidation and reduction of different metal ions.

CO4: To give the knowledge of properties and application of lanthanides and actinides.

Contents:

Unit I: Symmetry and Structure

Symmetry elements & symmetry operations, symmetry planes & reflections, inversion. Proper axis & proper rotation, improper axis & improper rotations, group of very high symmetry, classifications of molecules & illustrative examples. Molecular symmetry for compound having coordination number 2 to 9. Representative and matrix representations of operations. Reducible and irreducible representations. The great orthogonality theorem and its consequences. Character tables. Representations of vibrational modes in nonlinear molecules. Selection rules for vibrational absorption- complementary character of IR and Raman spectra, determination of the number of active IR and Raman lines. Applications to chemical bonding, construction of hybrid orbitals (BF_3, CH_4, PCl_5), transformation properties of AOs. Application to MO theory of H_2O, NH_3 and octahedral complexes

Unit II: Chemistry of d-block elements

Definition and General Characteristics of Transition Metals, Oxidation state, Comparisons of First and Second and Third transition Series. Important Chemistry with reference to

(i) Polyoxometallates and heteropolyoxometallates of Mo and W.

(ii) Intermolecular charge transfer complex: Cruetz-Taube ion; tungsten bronze and ruthenium red.

(iii) Metal Carbonyls: Bonding and structure. Carbonyl Clusters-synthesis, Heteroatoms in clusters, Electron counting in medium size clusters, capping rule.

(iv) Dinitrogen and Nitrosyls complexes: Bonding and structure.

(v) Non-Carbonyl Clusters-halide clusters, Multiple Metal –Metal bonds, quadruple bonds.

Unit III: MAGNETIC PROPERTIES OF TRANSITION METALS

Study of different types of magnetic behavior, measurement of magnetic susceptibility using Gouy and Faraday methods, spin-orbit coupling, quenching of orbital angular momenta, temperature-independent paramagnetism, spin crossover, application of crystal field theory to explain magnetic properties.

.**Unit IV: Oxidation and reduction:**

Standard potential and spontaneity, Nernst equation, Influence of pH, Disproportionation and Comproportionation, influence of complexation, relation between solubility and standard potentials. Latimer diagrams, Frost diagrams, Pourbaix diagrams, Application in environmental chemistry: natural waters, Chemical extraction of elements-chemical reduction, oxidation and electrochemical extraction.

Unit V: The f-block elements-Lanthanides and Actinides.

Electronic Configuration, Occurrence and recovery, General trends. Electronic, Optical and Magnetic properties. Coordination and organometallic compounds. Magnetic properties of Lanthanides and Actinides.

Suggested Readings

MSC 201: INORGANIC CHEMISTRY II

Books/References

1. P. Atkins, T. Overton, J. Rourke, M. Weller & F. Armstrong, Shriver and Atkins' Inorganic

Chemistry, Oxford University Press (2006). 2. F. A. Cotton. Chemical Applications of Group Theory, (3rd edn.), John Wiley & Sons (1999). 3. F. A. Cotton, G. Wilkinson, C. A. Murillo & M. Bochmann. Advanced Inorganic Chemistry (6th edition), John Wiley (1999).

4. J. E. Huheey, E. A. Keiter, R. L. Keiter& O. K. Medhi. Inorganic Chemistry: Principles of

Structure and Reactivity, Pearson Education (2006).

5. F. A. Cotton, G. Wilkinson, C. A. Murillo & M. Bochmann. Advanced Inorganic Chemistry (4th edition), John Wiley, 1993. 6. Principles of the Solid State, H. V. Keer, Wiley Eastern Limited, 2007 . 7. Inorganic and Organometallic Reaction Mechanisms (2nd Edition), Jim D. Atwood, Wiley – VCH 8. Inorganic Reaction Mechanisms, R. K. Sharma, Discovery Publishing House, 2007,

MSC 202: ORGANIC CHEMISTRY II **Marks: 30+70=100**
Total Credits: 4

Objective: **Students are introduced to important organic reactions, rearrangements along with oxidizing and reducing reagents. Students are also introduced to biocatalysis.**

Course Outcome: **Students will be able to understand and design organic reactions using appropriate reagents. Understand catalysis in biological systems involving enzymes and co-enzymes.**

CO1: To give the knowledge of organic name reactions and molecular rearrangement.

CO2: To give the knowledge of Oxidising reagents.

CO3: To give the knowledge of Reducing reagents.

CO4: To give the knowledge of organometallic reagents.

CO5: To give the knowledge of chemistry of enzyme and co-enzyme.

Contents:

Unit I: Study of Organic Name Reactions and Rearrangements
Mukaiyama Aldol condensation, Perkin reaction, Darzen condensation, Mannich reaction, Robinson Annulation, Stork-Enamine reaction, HVZ reaction, Simmon smith reaction, Baylis-Hillman, Nef reaction, Vilsmeier-Heck, Suzuki reaction, Heck reaction, Sonogashira coupling, Stille coupling, Ullmann coupling, Ring Opening and Ring Closing Metathesis-Grubb's (RCM) reactions.
Introduction to Molecular Rearrangement. Rearrangements to Electron deficient carbon: Wagner-Meerwein, Pinacol-pinacolone, Benzil-Benzilic acid, Arndt-Eistert synthesis. Rearrangements to Electron deficient nitrogen: Hoffman rearrangement, Curtius rearrangement, Schmidt and Lossen rearrangement, Beckmann rearrangement. Rearrangements to Electron rich carbon: Favorskii, Neber, Wittig, Stevens.

Unit II: Organic Reagents I
Cr and Mn oxidations: Oxidation of alcohols and aldehydes with Cr (VI) and Mn(VII) oxidants; oxidation of C=C and C-H bonds; uses of PCC, PDC, PFC and Collin's reagents. Peroxy oxidations: Alkene epoxidation by peracids and metal/alkyl hydroperoxides. Other methods of oxidations; DMSO and Swern oxidations; Oppenaur oxidatoion, Prevost and Woodward hydroxylation of alkenes, oxidative cleavage of C-C single and double bonds, periodates, LTA, oxidation of organic substrates with mercuric acetate and SeO_2, Dess-Martin periodinane oxidation.

Unit III: Organic Reagents II

a. Reductions: Reduction Methods (hydrogenations, complex metal hydride reductions, dissolving metal reductions, other metal & nonmetal based reductions, organic reagents based reduction methods) Catalytic hydrogenation, Pd/C, PtO_2, H_2/catalyst, (stereochemistry and mechanism), Wilkinson's catalyst, Boranes and Hydroboration reactions, $NaBH_4$, $NaCNBH_3$, $Na(OAc)_3BH$, LAH, DIBAL, superhydrides, R_3SiH, Bu_3SnH, NH_2NH_2, MPV reduction, etc. reductions of conjugated systems, Birch reduction, reductive fission of alcohols, Pinacol coupling, McMurry coupling, deoxygenation of alcohols and carbonyl compounds such as Wolff Kisner, Shapiro reaction, Bamford-Stevens reaction, Clemmensons reduction.

b. Organometallic compounds: Organo-magnesium, Organo-zinc and Organo-lithium, Sn reagents; Use of lithium dialkyl cuprate their addition to carbonyl and unsaturated carbonyl compounds.

Unit IV: Bio-organic chemistry I

Enzymes: Mechanism of enzyme action, different reactions catalyzed by enzymes, nomenclature, stereochemical aspects, cofactors, co-enzyme chemistry, structure and function of, CoASH, TPP, Lipoic Acid, NAD^+, NADH, FAD, $FADH_2$.

Suggested Readings

MSC 202: ORGANIC CHEMISTRY II

Text Books/Reference Books:

1. P. S. Kalsi. *Stereochemistry, Conformation and Mechanism* (7^{th} edn.), John Wiley (2008).

2. Stereochemistry of Organic Compounds: Principles and Applications by Nasipuri, John Wiley and Sons (6^{th} edn) (2009)

3. L. A. Paquette, Modern Heterocyclic Chemistry, John Wiley, (2007)

4. Reagents in organic synthesis-(John Wiley) Fieser and Fieser (2008)

5. Some modern methods of Organic synthesis-(Cambridge) W. Carruthares. (4^{th} edn) (2004)

6. Advances in Organometallic Chemistry- (A.P.) F. C. A. Stone and R. West. (2008)

7. Stereochemistry of Organic Compounds by Eliel & Wilen, John Wiley & Sons (2011)

8. T.L. Gilchrist, Heterocyclic Chemistry Longman (2010)

9. Heterocyclic Chemistry: Synthesis, Reactions and Mechanisms by R.K. Bansal, Wiley Eastern Ltd. (2009)

10. Synthetic approaches in organic chemistry by Raj K. Bansal, Wiley Eastern Ltd. (2010)

11. Gould E.S., Mechanism and Structure in Organic Chemistry, (2008).

12. Principles of organic synthesis-(Methuen) R. O. C. Norman (2010)

13. Organic Synthesis-(Prentice Hall)R. E. Ireland. (2011)

14. Modern synthetic reactions-(Benjamin) H. O. House. (2007)

15. J. Clayden, N. Greeves. et. al Organic Chemistry , Oxford Univ. Press, (2012) 4^{th} Edition.

MSC 203: PHYSICAL CHEMISTRY II **Marks: 30+70=100**

Total Credits: 4

Objective: To understand the fundamentals of Solid state and Statistical thermodynamics and Surface chemistry. Also included the advance topics of Chemical kinetics.

Course Outcome: Students will be able to explain the properties of different solids and their structure. Also apply the statistical thermodynamics to different ideal and real systems. Students will understand the basic concepts in surface chemistry.

CO1: To give the knowledge of structure and properties of solids.

CO2: To give the knowledge of kinetic study of enzymatic and fast reactions.

CO3: To give the knowledge of different distribution laws and their statistical thermodynamic studies.

CO4: To give the knowledge of adsorption study and colloidal properties.

CO5: To give the knowledge of chemistry of surfactants.

Contents:

Unit I: Solid State

Structure of solids: close packing of atoms, density of cubic crystals, structure of binary and ternary compounds; octahedral and tetrahedral voids, radius ratio rule, structure of ionic crystals; MX type crystals, MX_2 type crystals, specific defect structures.

Crystal structures: Crystal planes and Miller indices, Bragg's law and applications, Debye-Scherrer powder method, crystal defects, point defects-Schotky defect, Frenkel defect, metal excess defect, calculations of number of defects.

Electrical properties of solids: Free electron theory; Fermi energy, energy distribution function, electrical conductivity of metals, Band theory: conductors, insulators and semiconductors, the Hole, Fermi level in semiconductors, properties of semiconductors.

Unit II: Chemical Kinetics II

Effect of ionic strength, Kinetic salt effect. Enzyme catalysis and Michaelis-Menton Mechanism, Lineweaver Burk and Eadie plots, enzyme inhibition.

Treatment of unimolecular reactions: Lindemann theory and limitations, Lindemann-Hinshelhood, RRK and RRKM theories, electron transfer reactions.

Fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis, nuclear magnetic resonance method. kinetic isotopic effect.

Unit III: Statistical Thermodynamics

Configuration and weights, probability and the most probable configuration. Stirling Approximation. Canonical, grand canonical and microcanonical ensembles, Ensemble average and time average of property, corresponding distribution laws.

Boltzmann relation between thermodynamic probability and entropy. Partition functions: Calculation of translational, rotational, vibrational and electronic partition functions. Relation of partition functions with thermodynamic functions and equilibrium constants.

Thermodynamic properties of monatomic and diatomic gases (Seckur-Tetrode equation)-calculation of partition functions, thermodynamic function, principles of equipartition, theories of heat capacities (Einstein model and Debye modification), residual entropy.

Statistical thermodynamics of Ortho and Para hydrogen, Fermi-Dirac statistics, distribution law and applications to metals. Bose-Einstein statistics, distribution law and application to helium.

Unit IV: Surface Chemistry

Surface tension and surface free energy, capillary action. Pressure across an interface: Laplace equation, Kelvin equation; Wetting: Young-Dupre equation. Adsorption in liquid systems: Gibbs adsorption isotherm. Adsorption on solids: Langmuir isotherm, BET isotherm.
Sols, properties of sols, sols of surface active reagents, electrical properties of colloidal systems, coagulation of colloidal sols, electrokinetic properties, electro-osmosis, size determination of colloidal particles.
Surfactants, classification of surfactants, hydrophobic interaction, aggregation /micellization of surfactants, solubilization, critical micelle concentration (cmc), reverse micelles, factors affecting the cmc, microemulsion.

Suggested Readings

MSC 203: PHYSICAL CHEMISTRY II

Text Books/Reference Books:

1. Solid State Chemistry, D.K. Chakrabarty, New Age International Publishers, 2010.
2. Principles of Solid State Chemistry, H.V. Keer, New Age International Publishers Ltd., 2007.
3. Physical Chemistry (Vol.1 & 2), K.L. Kapoor, Macmillan, 2001.
4. Atkins Physical Chemistry, Peter Atkins and Julio D Paula, Oxford University Press, 2006.
5. Chemical Kinetics, Keith J. Leidler, Pearson, 2003.
6. Thermodynamics for Chemists, Samual Glasstone, East West Press, 2008.
7. Chemical Thermodynamics: Classical, Statistical and Irreversible, J. Rajaram, Pearson, 2013.
8. Statistical Thermodynamics, Andrew Maczek, San Val, 1998.
9. Statistical Thermodynamics, M.C. Gupta, New Age International Publishers Ltd., 2007
10. Surfactants and Interfacial Phenomena, M. J. Rosen, John Wiley & Sons, 1989
11. Micelles: Theoretical and Applied Aspects, Y. Moroi, Plenum, 1992.
12. Chemical Kinetics: The study of reaction rates in solution, Kenneth A Corners, VCH, 1990.
13. Physical Chemistry, R.S. Berry, S.A. Rice, J. Ross, Oxford University Press, 2nd eds., 2000.
14. Principles of Physical Chemistry, B.R. Puri, L.R. Sharma, Madan S. Pathania, Vishal Publishing Company, 2008.
15. Advanced Physical Chemistry, Gurdeep Raj, Krishna Prakashan Media (p) ltd, 2011.

MSC 204: Quantum Chemistry and Molecular Spectroscopy II **Marks: 30+70=100**
Total Credits: 4

Objective: **To provide fundamentals of quantum chemistry and molecular spectroscopy with respect to resonance techniques.**

Course Outcome: **Students will be able to understand the theoretical basis of Quantum chemistry and spectroscopic techniques of electronic, esr and nmr spectroscopy.**

CO1: To give the knowledge of quantum chemistry of hydrogen and hydrogen like ions.

CO2: To give the knowledge of different theories of quantum chemistry.

CO3: To give the knowledge of electronic transitions and their application.

CO4: To give the knowledge of ESR and Mossbauer spectroscopy.

CO5: To give the knowledge of NMR Spectroscopy.

Contents:

A. Quantum Chemistry

Unit I Hydrogen Atom

Rigid rotator model of rotation of diatomic molecule. Schrödinger equation, transformation to spherical polar coordinates. Separation of variables. Spherical harmonics. Discussion of solution. Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part, quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus.

Unit II Born-Oppenheimer Approximation and Approximate Methods

Born-Oppenheimer approximation, product wave-functions, complete many electron wave functions including electron spin, Pauli's anti-symmetry and exclusion principles

Variation theorem and Perturbation theorem. Time independent Perturbation theory for non-degenerate systems (upto second order in energy)

Huckel molecular orbital theory: postulates, application to ethane, butadiene, benzene

B. Molecular Spectroscopy

Unit III: Electronic Spectroscopy:

Electronic Transitions: The Frank-Condon Principle, ground and excited states of diatomic molecules, selection rule on the basis of symmetry properties of electronic states. Dissociation and pre-dissociation. Rotational fine structure, laser and laser spectroscopy, pump-probe spectroscopy, d-d and charge transfer spectra, change of molecular shape upon excitation. Fluorescence, phosphorescence, chemiluminescence and electroluminescence.

Unit IV: ESR Spectroscopy and Mössbauer spectroscopy

Basic principles of ESR spectra, line shapes and line widths. The g-values and hyperfine interaction, contact and dipolar mechanism. Spectra of simple organic radicals.

Introduction of Mössbauer effect, isomer-Shift, magnetic hyperfine interactions. Quadrupole moment. Electric field gradient. Quadrupole splitting. Applications in structure determination.

Unit V: NMR Spectroscopy

Nuclear spin, Langmor frequency, population of nuclear spin. Principle of NMR spectroscopy. Spin-Spin and spin-lattice relaxation. Origin of chemical shift. Spin-spin coupling. NMR of spectra of simple organic molecules. ^{13}C-NMR spectroscopy. Introduction to MRI of living system.

Suggested Readings

MSC 204: Quantum Chemistry and Molecular Spectroscopy II

Text Books/Reference Books:

1. Introductory Quantum Chemistry, A. K. Chandra. Tata McGraw Hill,1994.
2. Quantum Chemistry, I. N. Levine, Prentice Hall India, 2001.
3. Quantum Chemistry, By B K Sen.
4. Fundamentals of Molecular Spectroscopy by Colin N. Banwell & Elaine M. McCash (4^{th} edn) 2009 Published by Tata McGraw-Hill Publishing Company Ltd.

MSC 205: Inorganic Chemistry Practical **Marks: 30+70=100**
Total Credits: 4

Outcome: **To provide practical knowledge of inorganic synthesis and characterization using various techniques. Also practical knowledge of quantitative analysis.**

Course Outcome: **Students will be able to synthesize ligands and complexes and interpret the spectra and analyse ores and alloys.**

CO1: Practical knowledge of quantitative estimation.

CO2: Practical knowledge of qualitative analysis.

CO3: Practical knowledge of synthesis of various complexes.

CO 4: Practical knowledge of analysis of Ores.

CO5: Practical knowledge of characterization and analysis of synthesized complexes.

Contents:

1. Quantitative estimation involving titrimetric estimation-redox and complexometric, gravimetric and spectrophotometric methods in three component mixture/alloys.

2. Analysis of ore/alloys, cement and steel. Ores: Hematite, limestone, dolomite, cement, pyrolusite, etc. Alloys: Brass, Gunmetal, Bronze, Steel and other alloys.

3. Preparation and Characterization of the following compounds (at least 8 preparations are to be completed by turn): Characterization of Complexes by conductance measurements, infrared, UV-Visible and ^{1}HNMR Spectroscopy.

a) Reinecke salt

b) Potassium Tris(oxalato) manganese(III)

c) Potassium Tris(oxalate) Cr(III)

d) Tris(acetylacetonato) Al(III)

e) Bis(N,N-diethyldithiocarbamato)nitrosyliron(II)

f) Optical isomers of tris(ethylenediamine)cobalt(III)chloride

g) Linkage isomers of nitro and nitrito-pentamminecobalt(III) chloride

h) Tri(acetylacetonato)manganese(III)

i)Preparation of $[Fe(HY)H_2O].H_2O$(H_4Y=EDTA) and Dinitrogen Complex.

j) Any other suitable complex preferably of either Macrocyclic ligands or Schiff base.

Suggested Readings

MSC 205: Inorganic Chemistry Practical

Text Books / Reference Books:

1. *Advanced Practical Inorganic Chemistry*. Gurdeep Raj, Goal Publishing House, 2005.

2. Vogels Text Book of Quantitative Analysis. J. Mendahan, R.C. Danney and J.Mendhan, ELBS, 5th Ed, 2009.

3. *Practical Inorganic Chemistry*. G. Marr and B.W Rockett, Van Nostrand, 2001.

4. *Practical Inorganic Chemistry*. G. Pass and H. Sutcliffe, 2nd Ed, Chapman & Hill 2009.

5. *Inorganic Synthesis*. G.W. Parshall , Vol. 15, McGraw Hill, 2007.

MSC 301: INORGANIC CHEMISTRY III **Marks: 30+70=100**
Total Credits: 4

Objective: **Knowledge of inorganic reaction mechanism and organometallic chemistry**

Course Outcome: **Interpretation and factors controlling inorganic reactions, detailed knowledge of organometallic chemistry and applications.**

CO1: To give the knowledge of kinetics and reaction mechanisms of transition metal complexes.

CO2: To give the knowledge of organometallic compounds of transition metals.

CO3: To give the knowledge of reaction mechanism of organometallic compounds.

CO4: To give the knowledge of application of catalysis by organometallic compounds.

CO5: To give the knowledge of application of catalysis by selected organometallic compounds

Contents:

Unit I: Reaction Mechanism of Transition Metal Complexes

Complex formation in solution: Stability constants -overall and stepwise, factors affecting stability, Irving-Williams series, chelate and macrocyclic effects, steric effects and electron delocalization. Inert and labile complexes

Kinetics and mechanisms of octahedral substitution, acid hydrolysis, base hydrolysis- conjugate base mechanism, anation reactions, substitution reactions in square planer complexes, the trans effect, mechanism of substitution reaction. Electron transfer reactions- outer- and inner-sphere mechanisms.

Unit II: Organometallic Compounds of Transition metals:

MO theory and electron count rules for different types of organometallic compounds, synthesis, structure and bonding- alkyls, carbenes, carbynes and nonaromatic alkenes and alkynes, metallocenes, hapticity, multidecar compounds, phosphine and N-heterocyclic carbenes. Fluxional organometallic compounds. Different methods for characterization of organometallic compounds.

Unit III: Reactivity of Organometallic compounds

Organometallic reaction mechanisms -ligand substitution, oxidative addition, reductive elimination, Migration, insertion and deinsertion reactions and carbene involvement in metathesis and polymerization. Nucleophilic and electrophilic attack of coordinated ligands.

Unit IV: Organometallic Compounds in Catalysis.

Organometallic reagents in homogeneous catalytic reactions -hydrogenetion, Fischer-Tropsch reaction, water gas-shift reaction. Wacker oxidation, hydroformylation, carboxylation, Monsanto acetic acid synthesis and Polymerization, Asymmetric oxidation, Pd-catalysed C-C bond formation reactions, activation of small molecules by coordination.

Suggested Readings

MSC 301: INORGANIC CHEMISTRY III

Text Books/Reference Books:

1. Inorganic Chemistry, G. L. Meissler and D. L. Tarr, 3rd. Edition, Pearson.

2. Advanced Inorganic Chemistry by F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann. , Wiley 6th Edition.

3. Inorganic Chemistry Principles of structure and Reactivity by J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi; Pearson , 4th Edition.

4. Inorganic Chemistry, Weller, Overton, Rourke and Armstrong. Oxford Pub. (2015) 6th Edition.

5. Organometallic chemistry Vol I and II, M. Bochmann, Oxford

6. Applied organometallic chemistry and catalysis by R. Whyman, Oxford University press, (2001)

7. Heterogeneous catalysis, D. K. Chakrabartty and B. Vishanathan, New age Pub. 2008.

8. Organometallics by Eichenbroich Christoph,3rd Ed, Wiley VCH

9. The Organometallic Chemistry of Transition metals, by Robert Crabtree, 6th Ed. Wiley. Inorganic reaction mechanism by Basalo and Pearson.

MSC-302: ORGANIC CHEMISTRY III **Marks: 30+70=100**
Total Credits: 4

Objective: **Students are introduced to heterocyclic compounds bio-organic compounds; amino acids, peptides, proteins and carbohydrates along with bio energetic. Students are also introduced to photo chemistry and pericyclic reactions.**

Course Outcome: **Students learn about the properties of various types of bio-molecules and interpret various biological processes. Knowledge of photochemistry and pericyclic reactions will enable students to handle problems associated with these processes.**

CO1: To give the knowledge of structure and reactivity of heterocyclic compounds.

CO2: To give the knowledge of preparations and reactions of bioorganic compounds.

CO3: To give the knowledge of application of photochemistry in some organic compounds.

CO4: To give the knowledge of pericyclic reactions and molecular rearrangements.

CO5: To give the knowledge on metabolism processes involving living organisms.

Contents:

Unit I: Chemistry of Heterocyclic compounds

Nomenclature of heterocyclic compounds. Structure, reactivity, synthesis and reactions: pyridine, quinoline, isoquinoline, indole, benzofuran, benzothiophene, pyrazole, imidazole, oxazole, isoxazole, thiazole, isothiazole, pyridazine, pyrimidine and pyrazine.

Unit II: Chemistry of amino acids, peptides and proteins

Classification of amino acids, methods of preparations, reactions of amino acids. Isoelectric point of amino acids and its determination. Absolute configuration of amino acids. Peptides: peptide linkage, nomenclature of polypeptides, general principles of polypeptide synthesis, protection of amino and carboxylic groups. Determination of structure of peptides. Proteins: General properties, classification and detection of protein. Primary, tertiary, secondary and quaternary structures of proteins. Biosynthesis of amino acids.

Unit III: Photochemistry & Pericyclic Reactions

A. Photochemistry- Cis-trans isomerisation, Norrish type I & II reaction, Paterno-Buchi reaction, photoreduction of Ketones, dipimethane rearrangement, photochemistry of arenes, Barton reaction.

B. Pericyclic reactions**-**Main features of pericyclic reactions; Woodward-Hoffman rules, correlation diagram and FMO approaches; Electrocyclic reactions – conrotatory and disrotatory motions for *4n* and *4n+2* systems. Cycloadditions– antarafacial and suprafacial additions, [2+2]

and [4+2] reactions, 1,3-dipolar cycloadditions and chelotropic reactions; Sigmatropic *[i,j]* shifts of C-H and C-C bonds; Sommelet-Hauser, Claisen, thio-Claisen, Cope and aza-Cope rearrangements.

Unit IV: Bioorganic Chemistry II

A. Characteristics and properties of carbohydrates, monosaccharides, open chain and ring structure, Haworth and conformational representations, oxidation, determination of ring size, glycosides, anomeric effect; Oligosaccharides and Polysaccharides - sucrose and other oligosaccharides, starch, cellulose and other polysaccharides.

B. Energy generation in living systems, metabolism of carbohydrate (Glucose), glycolysis and Kreb's cycle, Standard free energy change in biochemical reactions. ATP as biochemical currency, ATP-ADP cycle. cell membrane. transmembrane potential, active transport of ions through cell membranes, membrane equilibrium, muscular contraction.

Suggested Readings

MSC-302: ORGANIC CHEMISTRY III

Text Books/ Reference Books

1. Organic Chemistry: by I. L. Finer (Part I & II), Longman Group Ltd. (6^{th} edition), (2009)
2. Lehniger Principles of Biochemistry by David L. Nelson & Michael M. Cox, Macmillan Worth Publishers (2011)
3. Organic Chemistry of Natural Products (Vol. I & II) by Gurdeep R. Chatwal, Himalaya Publishing House. (2013)
4. Pericyclic reactions: a mechanistic study by S.M. Mukherji, Macmillan Co. of India Ltd (2011)
5. Pericyclic reactions by Ian Fleming, Oxford Chemistry Primers, (2^{nd} edition), (2015)

MSC-303: PHYSICAL CHEMISTRY III **Marks: 30+70=100**

Total Credits: 4

Objective: **The course is directed to understand fundamentals of photochemistry, Dynamic electrochemistry and Catalysis**

Course Outcome: **Through this course students will acquire detailed knowledge on different photochemical processes, advanced electrochemistry and catalysis**

CO1: To give the knowledge of photophysical phenomena and its applications.

CO2: To give the knowledge of dynamic electrochemical theory.

CO3: To give the knowledge of theories of electrified interface.

CO4: To give the knowledge of thermodynamics of electrified interface.

CO5: To give the knowledge of classification of catalysis and their application.

Contents:

Unit I: Photochemistry

Photo physical phenomena: mechanism of absorption and emission phenomena- Einstein's treatment. Electronic structure of molecules, electronically excited singlet states, designation based on multiplicity rule, life time of electronically excited state, construction of Jablonski diagram, electronic transitions and intensity of absorption bands, photophysical pathways of excited molecular system, prompt fluorescence, delayed fluorescence (E-type and P-type delayed emission), phosphorescence, fluorescence quenching: concentration quenching, quenching by excimer and exciplex emission, Stern-Volmer relation, critical energy transfer distances, energy transfer efficiency. Chemiluminescence, Photocatalysis, Photosensitization, Photodynamic therapy of tumor.

Unit II: Dynamic Electrochemistry **12 hrs**

Ion-solvent interactions, the Born model, thermodynamic parameters of ion-solvent interactions, Debye-Huckel theory of ion-ion interactions, extended Debye-Huckel equation, Debye Huckel limiting law, Debye-Huckel-Onsagar treatment and its extension to ion-solvent interactions. Debye-Huckel-Bjerrum model. The random walk model of ionic diffusion-Einstein Smoluchowski reaction.

Unit III: Electrified Interface

Polarizable and nonpolarizable interfaces, Thermodynamics of electrified interface equations. Derivation of electro-capillarity, Lippmann equations (surface excess), methods of determination.

Unit IV: Theories of Electrified Interface 5 hrs

Structure of electrified interfaces. Helmholtz, Guoy-Chapman, Stern and Devanathan models.

Unit V: Catalysis 12 hrs

Catalysts, classification of catalysts. Characterization of catalysts: methods of surface analysis, surface area, pore size, void fraction, particle size, mechanical strength, surface chemical composition, surface acidity and reactivity.

Phase transfer catalysts, Heterogeneous catalysts, mechanism and kinetics of heterogeneous catalysis-Langmuir-Hinshelwood model, Eley-Riedel model) shape and size selectivity of catalysts. Clays and zeolites.

Suggested Readings

MSC-303: PHYSICAL CHEMISTRY III

Text Books/Reference Books:

1. Fundamentals of Photochemistry, K.K. Rohtagi-Mukherjee, New Age International, New Delhi, 1986.

2. Photochemistry, J.G. Calvert and J.N. Pitts, Jr., John Wiley & Sons, New York, 1966.

3. Principles and Applications of Photochemistry, R.P. Wayne, Oxford Univ. Press, 1988.

4. Principles of Fluorescence Spectroscopy, 2nd Ed., J.F.L. Lakowicz, Plenum Pub., New York, 1999.

5. Modern Electrochemistry: An Introduction to an Interdisciplinary Area, Amulya K.N. Reddy, John O. Bockris, Springer, 2000.

6. Modern Electrochemistry 1: Ionics, John O. Bockris, A.K.N. Reddy, Springer, 1998.

7. Heterogeneous Catalysis, D. K. Chakrabarty, B. Viswanathan, New Age Int., 2008.

MSC-304: Applications of Spectroscopy **Marks: 30+70=100**
Total Credits: 4

Objective: **The course is directed to understand different spectroscopic techniques.**

Course Outcome: **students will be able to elucidate the chemical structure of unknown compounds.**

CO1: To give the knowledge of characterization of organic molecules by Infra Red spectroscopy.

CO2: To give the knowledge of fragmentation pattern and application by mass spectroscopy.

CO3: To give the knowledge of nuclear magnetic resonance spectroscopy and its application.

CO4: To give the knowledge on 2D NMR.

CO5: To give the knowledge of spectroscopic technique structural elucidation.

Contents:

Unit I**: Infrared Spectroscop**y
Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines; detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acid anhydrides, lactones, lactams, conjugated carbonyl compounds); effects of H-bonding and solvent effect on vibrational frequency, extension to various organic molecules for structural assignment.

Unit II**: Mass Spectrometry**
Mass spectral fragmentation of organic compounds, common functional groups; molecular ion peak, fragmentation *via* retro-Diels-Alder reaction, McLafferty rearrangements, examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Unit III**: Nuclear Magnetic Resonance Spectroscop**y
Approximate chemical shift values of various chemically non-equivalent protons and correlation to protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic); coupling constants; protons bonded to other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides, SH); chemical exchange, effect of deuteration; complex spin-spin interaction between two, three, four and interacting nuclei (first order spectra); complex interaction, virtual coupling, stereochemically hindered rotation, Karplus curve, variation of coupling constant with dihedral angle, nuclear magnetic double resonance, simplification of complex spectra using shift reagents, Fourier transform technique and Nuclear Overhauser Effect (NOE).

C-13 NMR:Basic difference with ^{1}H NMR, Chemical shift (aliphatic, olefinic, alkynes, aromatic, hetero-aromatic, carbonyl carbon); two-dimensional NMR spectroscopy, NOESY, DEPT and INEPT terminologies.

Unit-IV**:Applications**

Structure elucidation of organic compounds using multiple spectroscopic data (NMR, MS, IR and UV-Vis).

Suggested Readings

MSC-304: Applications of Spectroscopy

Textbooks / Reference Books:

1. R. M. Silverstein, G. C. Basseler& T. C. Morill. *Spectroscopic Identification of Organic Compound*s, John Wiley 7thedn (2005).

2. W. Kemp. *Organic Spectroscopy* (6thedn.), McMillan Press Ltd. (2009).

3. Introduction to Spectroscopy by D.L. Pavia, G. M. Lampman, G. S. Kriz, Harcourt College Publisher, NY, 2001

4. D Williams & I. Fleming. *Spectroscopic Methods in Organic Chemistr*y, McGraw Hill (2010).

5. C. N. Banwell& E. M. McCash. *Fundamentals of Molecular Spectroscop*y, Tata McGraw-Hill, New Delhi (2006).

MSC 305: Physical Chemistry Practical **Marks: 30+70=100**

Total Credits: 4

Objective: **This is a core laboratory course introducing some experimental physical chemistry. The objective of the course is to introduce experiments on chemical kinetics, electrochemistry and spectroscopy etc.**

Course Outcome: **From this course, the students will understand physical chemistry from experimental point of view. Moreover, they will learn some modern methods of analysis required in different areas of research.**

CO1: Practical knowledge of study of kinetics.
CO2: Practical knowledge on equilibrium reactions and phase studies
CO3: Practical knowledge of viscosity and surface tension study.
CO4: Practical knowledge of conductometric and pH metric titration of mixture of component.
CO5: Practical knowledge of spectroscopic analysis.

Contents:

A. Chemical Kinetics:

1. Determine the constant of hydrolysis of methyl acetate catalysed by an acid and the energy of activation using least square method.
2. Determine the relative strength of two acids by studying the hydrolysis of methyl acetate.
3. Study the hydrolysis of methyl acetate catalysed by HCl and equinormal solution of urea hydrochloride, and hence determines the degree of hydrolysis of the salt.
4. Study the kinetics of the reaction between iodine and acetone in acidic medium by half-life period method and determine the order with respect to iodine and acetone.
5. Study the saponification of ethyl acetate by sodium hydroxide and determine the order of reaction and energy of activation.
6. Study the inversion of cane sugar in presence of two acids and determine the relative strengths of the two acids.
7. Study the kinetics of the reaction between hydrogen peroxide and hydrogen iodide**.**

B. Distribution law:

8. Determine the distribution coefficient of iodine between CCl_4 at a given temperature.
9. Determine the equilibrium constant of the reaction $KI + I_2 \overset{k}{\Leftrightarrow} KI_3$ by distribution method.

C. Viscocity:

10. Study the variation of viscosity of gycerol with temperature, and determine the temperature coefficient of viscosity of nitrobenzene.
11. Determine the molar mass of a polymer by viscometric method.

D. Surface Tension:

12. Determine the limiting cross-section area of n-propyl alcohol by surface tension measurements.

13. Determine the critical micelle concentration of sodium dodecyl sulphate in aqueous medium by surface tension measurements.

E. Conductivity:

14. Determine the equivalent conductivity of acetic acid at infinite dilution by Kohlrausch's method and determine the degree of hydrolysis of the acid.

15. Determine the relative strength of chloroacetic acid and acetic acid by conductance measurements.

16. Determine the solubility and solubility product of $PbSO_4$ at room temperature by conductance measurements.

F. pH-metry:

17. Determine the strength of the components of the mixtures: (i) HCl and acetic acid, (ii) H_2SO_4 and $CuSO_4$.

18. Determine the amount of components of the following mixtures: (i) HCl and acetic acid, (ii) HCl and oxalic acid, (iii) KCl and KBr and KI.

19. Determine potentiometrically the strengths of solutions of HCl and acetic acid individually and a mixture of the two using standard NaOH solution.

20. Titration of ferrous ammonium sulphate against potassium dichromate and determine the standard electrode potential of the ferrous/ferric system.

G. Spectrophotometry:

21. Varify Beer's law and determine the concentration of solutions KMnO4/$K_2Cr_2O_7$.

22. Determine the composition of iron-salicylic acid complex spectrophotometrically by Job's method of continuous variation.

Suggested Readings

MSC 305: Physical Chemistry Practical

Text Books / References Books:

1. Advanced Practical Physical Chemistry by J.B. Yadav, KRISHNA Prakashan Media (P) Ltd, 2012.
2. Experimental Physical Chemistry by R.C. Das, B. Behera, Tata McGraw-Hill Publishing Company Limited.

MSC-306A: Environmental pollution and management **Marks: 30+70=100**

Total Credits: 4

Objective: Students will be introduced to the concerns/prospective about environmental. Students are expected to understand different aspects of environmental chemistry, chemistry of atmosphere, soil and water.

Course Outcome: Students will be able to demonstrate an understanding of environmental chemistry, viz. air, water and soil chemistry and waste management.

CO1: To give the knowledge of scope of environmental chemistry.
CO2: To give the knowledge of chemistry of organic and inorganic toxic materials.
CO3: To give the knowledge of water and air pollution.
CO4: To give the knowledge of soil pollution
CO5: To give the knowledge of waste management and recycling.

Contents:

Unit I: Concept and scope of Environmental Chemistry

Definition and explanation for various terms, segments of environment, natural cycles in the environments; hydrological cycle, carbon cycle, oxygen cycle and nitrogen cycle.

Unit II: Chemistry of organic and inorganic toxic materials

Introduction to chemical hazards and safety, hydrocarbons - chemistry of hydrocarbon decay, environmental effects, effects on macro and microorganisms, detergents, dyes, synthetic polymers, industrial wastes-some examples.

Unit III: Atmospheric pollution

Acid-rain, smog, industrial and vehicular pollution, ozone layer depletion, global warming and minimization of these problems.

Water pollution:

Eutrophication, ground water contamination with arsenic, fluoride, toxic heavy metals and remediation, drinking water contamination and water-borne diseases, sources of germs and prevention.

Unit IV: Soil pollution:

Soil pollution due to industrial disposal and use of chemicals including pesticides and synthetic fertilizers, remediation of agricultural lands.

Unit V: Waste management and recycling

Waste classification, solid waste management and disposal, ocean dumping, waste water treatment, sludge treatment, water reuse and recycling.

Suggested Readings

MSC-306A: Environmental pollution and management

Text Books / Reference Books:

1. Manahan, S.E. *Environmental Chemistry, 9th edn*., (CRC Press 2009).

2. De A K, Environmental Chemistry, New Age International Publishers.

3. Moore J. W. & Moore. E. A. *Environmental Chemistry, 2nd edn*., (Academic Press, New York 1985).

4. B.K. Sharma, & Kaur, H. *Environmental Chemistry,* (Goel Publishing House, Meerut, India, 1996).

MSC 306B: Green Chemistry **Marks: 30+70=100**

Total Credits: 4

Objective: Introduction to Green Chemistry and its principles. To apply Green chemistry to laboratory/industry.

Course Outcome: Students will be able to describe/compare relationships between Green Chemistry and chemical laboratory and industry, particularly in the design of safer chemicals and processes

CO1: To give the knowledge of introduction to green chemistry.
CO2: To give the knowledge of waste management.
CO3: To give the knowledge of catalysis and its application.
CO4: To give the knowledge of environmental pollution control.
CO5: To give the knowledge of prevention of waste

Contents:

Unit I: Introduction to Green Chemistry

Definition, goals, principles of green chemistry – prevention of waste, atom economy, less hazardous chemical synthesis, green solvents and designing of green synthesis.

Unit II: Waste: Production, problem and prevention

Introduction, some problems caused by waste, sources of waste, waste minimization

Unit III: Catalysis and Green Chemistry

Introduction to catalysis, heterogeneous and heterogeneous catalysts, phase transfer catalysis, bio-catalysis, photocatalysis, organo catalysts.

Unit IV: Controlling Environmental Performance

Environmental management systems, ISO 14001, The Europian Eco-management and audit scheme, eco-levels, legislation, integrated pollution prevention and control.

Suggested Readings

MSC 306B: Green Chemistry

Text Books / Reference Books:

1. Anastas, P T and Warner, J C Green Chemistry: Theory and practice, (Oxford University Press, 1998)

2. Lancaster, Mike, Green Chemistry: An Introductory Text, RSC, 2002.

MSC -401 A: NATURAL PRODUCT CHEMISTRY **Marks: 30+70=100**
Total Credits: 4

Objective: Students are introduced to various classes of natural products, their isolation, synthesis and bio-synthesis.

Course Outcome: Students will be able to identify various types of natural products, use their knowledge to identify newer material having important natural products.

CO1: To give the knowledge of introduction of natural products.

CO2: To give the knowledge of introduction to steroids and their synthetic route. alkaloids and terpenoids - their synthetic route.

CO3: To give the knowledge of introduction to alkaloids and terpenoids - their synthetic route.

CO4: To give the knowledge of classification of vitamins and its chemistry.

CO5: To give the knowledge of structure, synthesis and chemistry of nucleic acid.

Contents:

Unit I: Natural Products and their Biosynthetic Pathways
Classification of natural products, their isolation and characterisation; biosynthesis pathways for natural products using co-enzymes and enzymes; primary and secondary metabolites – fatty acid derivatives and related compounds, general biogenesis and synthesis of cis-jasmone, methyl jasmonate, prostaglandins, exaltone and muscone.

Unit II: Steroids
Nomenclature of steroids and synthesis of squalene; biosynthesis of diterpenes, higher terpenes and steroids; lanosterol and caretonoids; synthesis of equlenins; estrogens and total synthesis of non-aromatic steroids (progesterones); corticosteroids; degradation of diosgenin to progesterone and its synthesis; miscellaneous transformations of steroid molecules.

Unit III: Alkaloids and Terpenoids
General biosyntheses of mono- and sesquiterpenes, *trans*-chrysanthemic acid, cyclo-pentato monoterpene lactone, synthesis of α-vetivone, β-eudesmol, and Satonine; synthesis of abietic acid, *cis* juvenile hormone; *trans* annular cyclisation of caryophyllene, synthesis of caryophyllene, isocaryophyllene and longifolene; Synthesis and biosynthesis of common alkaloids: reticuline, morphine, yohimbine and tylophorine.

Unit IV: Vitamins

Classification of carotenoids, chemistry of β-carotene, lycopene and Xanthophiles. Provitamin A and food colouring properties of carotenes. Chemistry of thiamine, riboflavin, retinol, tocopherols, Vitamin C, pyridoxine, pentothenic acid and folic acid, role of Vitamins as co-enzyme.

Unit V: Nucleic Acids

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

Suggested Readings

MSC -401 A: NATURAL PRODUCT CHEMISTRY

Text Books/Reference Books:

1**.** Natural products: Chemistry and Biological significance – J. Madd, R. S. Davidson, J. B. Hobbs, D.V. Banthrope. (2011)

2**.** Organic chemistry, Vol 2., - I..L. Finar. (2011)

4**.** Chemistry, Biological and Pharmacacological properties of medicinal plants from the americas - Ed. Kurt, M. P. Gupta and A. Marston. (2009)

5**.** New trends in Natural product chemistry – Alta – Ur- Rahman and M.I. Choudhary. (2010)

MSC-402 A: MEDICINAL CHEMISTRY **Marks: 30+70=100**
Total Credits: 4

Objective: **Students are introduced to concept of medicinal chemistry, drug design, various classes of drugs, their mechanism of action and synthesis.**

Course Outcome: **Students learn about drug molecules and able to identify various classes of drugs used against specific diseases.**

CO1: To give the knowledge of introduction of drug, structure activity relationship and their mode of action.

CO2: To give the knowledge of introduction, classification and mode of action of antibiotics.

CO3: To give the knowledge of introduction, synthesis and mode of action of anesthetics, anti depressants.

CO4: To give the knowledge of synthetic route of some important drugs.

CO5: To give the knowledge of mode of action of some important drugs.

Contents:

Unit I: Introduction
Structure activity relationship (SAR), quantitative structure-activity relationship (QSAR); Factors affecting bioactivity – resonance, inductive effect, isosterism, bio-isosterism, spatial considerations; Theories of drug activity – occupancy theory, rate theory, induced fit theory Concept of drug receptors – elementary treatment of drug-receptor interactions; physicochemical parameters – lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials; factors affecting modes of drug administration, absorption, metabolism and elimination; significance of drug metabolism in medicinal chemistry.

Unit II: Antibiotics
Introduction. Inhibitors of β-lactam rings, antibiotics inhibiting protein synthesis; Isolation, structure elucidation, synthesis, SAR and mode of action of penicillins; synthesis of penicillin G, penicillin V, ampicillin, amoxicillin and cephalosporin. Isolation, structure elucidation, synthesis, SAR and mode of action of following antibiotics: streptomycin, tetracyclines and chloroamphanicol.

Unit III: Anaesthetics and Antidipressants
General Anaesthetics: Mode of action of: enflurane, isoflurane, halothane, cyclopropane, thiopentone sodium, ketamine, methohexetal sodium, medazolam, fentanyl, etomidate.
Local Anaesthetics: Mode of action of: cocaine, cyclomethaycaine sulphate, benzocaine, procaine hydrochloride, mepivacaine hydrochloride, bupivacaine hydrochloride, phenacaine hydrochloride, dyclonine, diperodone, lidocaine hydrocholoride, etidocaine hydrochloride.
Antidipressants: Mode of action of: isocarboxazid, tranylcypromine, dibenzazepines, dibenzocycloheptanes, doxepine, trazodone, fluoxetine.

Synthesis of: fentanyl, etomidate, cocaine, procaine hydrochloride, isocarboxazid, fluoxetine.

Unit IV: Old and New Drugs

i) **Anti- inflammatory**: Mode of action of: ibuprofen, oxyphenylbutazone, diclophenac, indomethacin. Synthesis of ibuprofen, diclophenac,

ii) **Antitubercular & antileprotic**: Mode of action of: ethambutol, isoniazid & dapsone. Synthesis of dapsone.

iii) **Antihistamines**: H_1-Receptor antagonists. Mode of action of: diphenhydramine. Cyclizine, ceterizine. Synthesis of diphenhydramine.

iv) **Tranquilizers**: Mode of action of: diazepam, trimeprazine. Synthesis of diazepam.

v) **Cardiovascular**: Synthesis of dilliazem, quinidine, methyldopa, atenolol, oxyprenol

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

Suggested Readings

MSC-402 A: MEDICINAL CHEMISTRY

Text Books/Reference Books:

1. Introduction to Medicinal Chemistry, A Gringuage, Wiley-VCH. (2009)

2. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed Robert F. Dorge. (2006)

3. An Introduction to Drug Design, S.S. Pandey and J.R. Dimmock, New Age International.(2008)

4. Burger's Medicinal Chemistry and Drug Discovery, Sixth Edition, Ed.M.E.vWolff, John Wiley. (2010)

5. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw-Hill. (2011)

6. The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.(2007)

7. Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley. (2008)

8. Pharmaceutical Substances., Kleemann, Vol-I & II., Fourth edition., Thieme. (2007)

9. Principles of Medicinal Chemistry., William Foye, Fourth Edition., Lippincott, William and Wilkins. (2005)

10. Analytical Profile of Drug Substances (Series)., Florey.,(2007)

11. Merck Index., Thirteenth edition., Merck & Co. (2010)

12. Total synthesis of Natural products, Apsimon (Series). (2007)

13. Principles of Medicinal Chemistry by S.S. Kadam, Mahadik, Bothera, Nirali Publication, 11 th edition. (2002)

14. Pharmacology and Pharmacotherapeutics by R.S. Satoskar, Bhandarkar, Popular Prakeshan. (2009)

15. Bio Pharmaceutics and Pharmacokinetics by Bhramankar, Valabh prakashan. (2004)

MSC-401 B: BIOINORGANIC AND INORGANIC PHOTOCHEMISTRY

Marks: 30+70=100
Total Credits: 4

Objective: **To provide knowledge of inorganic biomolecules and role in biological processes.**

Course Outcome: **Students will be able to interpret the chemistry of biological processes.**

CO1: To give the knowledge of concept of electron transfer mechanism.

CO2: To give the knowledge of introduction and mechanism of different catalysis and inorganic photochemistry.

CO3: To give the knowledge of Biological cycles, Sensors and Biominerals.

CO4: To give the knowledge of toxicity of metals and their complexes in therapeutic applications.

CO5: To give the knowledge of Inorganic Photchemistry.

Contents:

Unit I: Transport, transfer and transcription

The physical structure of Cells, the inorganic compound of living organisms. Sodium and Potassium transport, Calcium signaling proteins, Zinc in transcription, Selective transport and storage of iron, Oxygen transport and storage, Electron transfer.

Unit II: Catalytic processes:

Acid –base catalysis, Enzymes dealing with H_2O_2 and O_2, the reaction of cobalt-containing enzymes, Oxygen atom transfer by molybdenum and tungsten enzymes.

Unit III: Biological cycles, Sensors and Biominerals:

The Nitrogen cycle and Hydrogen cycle. Iron proteins as sensors, proteins that sense Cu and Zn levels. Common example of biominerals.

Unit IV: Therapeutic Applications and Toxicity of Metals:

The chemistry of elements in medicine. Anticancer drugs (platinum complexes). Antiarthritis drugs (gold, copper and its complexes). Bismuth in the treatment of gastric ulcers, Lithium in Bipolar disorders, Organometallic drugs in malaria treatment, Cyclams as anti-HIV agents, Chelation therapy, Imaging agents. Toxicity of metal ions.

Unit V: Inorganic Photochemistry

Introduction to inorganic photochemistry, photochemical laws, characteristics of electronically excited states of inorganic compounds, photochemistry of excited state redox reactions, photosensitization, photochemical reactions: substitution, decomposition, rearrangement and redox reactions. Inorganic photochemistry in biological processes and organometallic compounds.

Suggested Readings

MSC-401 B: BIOINORGANIC AND INORGANIC PHOTOCHEMISTRY

Text Books/Reference Books:

1. Inorganic Chemistry, Weller, Overton, Rourke and Armstrong. Oxford Pub. (2015)6th Edition.

2. Inorganic Chemistry, G. L. Meissler and D. L. Tarr, 3rd. Edition, Pearson.

3. Advanced Inorganic Chemistry by F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann. , Wiley 6th Edition.

4. Inorganic Chemistry Principles of structure and Reactivity by J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi; Pearson , 4th Edition.

5. The biological chemistry of elements by J. J. R. Frausto da Silva and R. J. P. Williams, Oxford University press (2001)

6. BioIological inorganic chemistry by R. R. Crichton, F. Lallemand, I. S. M. Psalti and R. J. Ward, Elsevier (2007)

7. Bioinorganic chemistry by K. Hussain Reddy, New Age Publisher (2007)

MSC-402 B: Materials Chemistry and Nanomaterials **Marks: 30+70=100**

Total Credits: 4

Objective: **To provide knowledge of frontier areas- material chemistry and nanomaterials.**

Course Outcome: **Students will be well-equipped to carry out research in frontier and challenging areas of material and nanoscience and their applications.**

CO1: To give the knowledge of material synthesis.

CO2: To give the knowledge of properties of hydrides and hydrogen storage material.

CO3: To give the knowledge on the synthesis of nanomaterials.

CO4: To give the knowledge of the structure and properties of nanomaterials

CO5: To give the knowledge of inorganic polymer and their application.

Contents:

Unit I: Synthesis of materials

Bulk material, Defects and ion transport-Extended defects, atom and ion diffusion, solid electrolytes. Metal oxides, nitrides and fluorides; Layered MS_2compounds and intercalation, Chevral phases. Framework Structures-based on tetrahedral oxoanions and linked octahedral and tetrahedral centres.

Unit II: Hydrides and Hydrogen storage materials

Metal hydrides and inorganic hydrogen –storage materials. Optical properties of inorganic materials-coloured solids, white and black pigments, photocatalysts. Semiconductor chemistry-Group 14 semiconductors, semiconductor systems isoelectronic with silicon. Molecular materials and fullerides-fullerides, molecular materials chemistry.

Unit III: Nanomaterials

Terminology and history, Synthesis-solution based, vapour phase, template synthesis and characterization.

Unit IV: Nanostructures and Properties

One dimensional control: carbon nanotubes and inorganic nanowires; Two-dimensional control: grapheme, quantum wells and solid-state superlattices. Three-dimensional control; mesoporous materials and composites. Special optical properties of nanomaterials.

Unit V: Inorganic polymers

(i) Silicon Polymers: organo silicon polymers, polysilanes, polysiloxanes. Synthesis and their uses. (ii) Boron Polymers: different boron polymers having B-H, B-N, B-P, B-B, B-O, B-Si and B-C bonds (polymers containing boron atoms in the backbone or in pendent groups). Various uses of boron containing polymers. (iii) Phosphazenes- cyclic and polymeric phosphazenes.

Suggested Readings

MSC-402 B: Materials Chemistry and Nanomaterials

Text Books/Reference Books:

1. Inorganic Chemistry 6th Edition, Weller, Overton, Rourke and Armstrong. Oxford Pub. 2015.

2. Solid state Chemistry, New Age Puublication, D. K. Chakrabortty 2010.

3. New Directions of Solid state chemistry, C. N. R. Rao and J. Gopalakrishnan, Cambridge University Press(1997)

4. NanoChemistry: a Chemical approach to nanomaterials, G.A. Ozin and A. C. Arenault. Spinger (2005)

5. Introduction to Nanotechnology, C. P. Poole and F. J. Owens, Wiley-Interscience(2003).

6. Inorganic nanoparticles: Synthesis, application and perspectives, Altavilla and E. Ciliberto, CRC press (2012).

7. Inorganic Polymers by H. Allock, J. E. Mark and R. West, 1992, Oxford University Press.

8. Inorganic nanowires: Application, Properties and Characterization. By M. Meyyappan, CRC Press (2012)

MSC-401 C: CHEMICAL DYNAMICS AND ELECTROCHEMISTRY

Marks: 30+70=100
Total Credits: 4

Objective: **The course deals with Chemical Dynamics and Advanced Electrochemistry including energy storage.**

Course Outcome: Students will be able to apply different theories concerning chemical dynamics and electrochemistry.

CO1: To give the knowledge of introduction to different theories use in reaction in solution.

CO2: To give the knowledge of molecular reaction dynamic and its application to quantum mechanical treatment.

CO3: To give the knowledge of electrode kinetic reactions.

CO4: To give the knowledge of electroanalytical and spectroelectrochemical technique.

CO4: To give the knowledge of introduction and classification of fuel cells and their applications.

Contents:

Unit I: Reactions in Solution

Cage effect, Reaction between gas phase and solution phase. Influence of solvent on reaction rates (double sphere model). Primary and secondary isotope effects on reaction rates. Linear Free Energy relationships (LFER): thermodynamic implications of LFER, inductive and electromeric effects on reaction rates, effect of substitutents on activation energies, Hammett and Taft equations, Swain-Scott and Edward equations, Winstein Grunwald relationship, isokinetic relationship-evaluation of isokinetic temperature and its significance, diffusion and activation controlled reactions.

Unit II: Molecular Reaction Dynamics

Reactions in flow systems, kinetics of fast reactions- flow methods, pulse methods- flash photolysis, pulse radiolysis, potential energy surface for $H+H_2$. Theoretical calculation of activation energies of potential energy surfaces, transmission co-efficient. Quantum mechanical

tunneling, Murcus theorem, reaction co-ordinate, symmetry numbers and statistical factors, mean free path, reaction rates and cross sections.

Unit III: Electrode Kinetics

Butler-Volmer equation, exchange currents, Tafel plot, overpotential, physical meaning of symmetry factor, Butler-Volmer equation for multistep reactions, high and low field approximation.

Unit IV: **Electroanalytical Techniques and Spectroelectrochemical techniques**

Voltammetry at a dropping mercury electrode (DME): principles of normal dc polarography, normal pulse polarography-differential pulse polarography-ac polarography. Applications of cathodic and anodic stripping voltammetry. Chronopotentiometry and Chronoamperometry. Impedance Spectroscopy, cyclic voltammetry: principle, experimental set up, electode used, quantitative analysis-determination of diffusion coefficients-diagnostic criteria for reversible, quasireversible and irreversible processes.

Unit V: Fuel Cells

Fuel cells: classification- alkaline fuel cells, solid polymer electrolyte fuel cells, phosphoric acid fuel cells, molten carbonate fuel cells and solid oxide fuel cells- brief description, reactions and applications of each type of fuel cell. Electrochemical supercapacitors: brief description, advantages and applications.

Suggested Readings:

MSC-401 C: CHEMICAL DYNAMICS AND ELECTROCHEMISTRY

Text Books / Reference Books:

1. Chemical Kinetics, 3rd Edition, K.J. Laidler, (Mc-Graw Hill Inc.) New York, 2007.

2. Kinetics and Mechanism, Frost and R.G.Pearson (John-Wiley) New York, 1962.

3. Introduction to Molecular Dynamics and Chemical Kinetics, G.D. Billing and Milkelson (Wiley Interscience), 1996.

4. Modern Electrochemistry – Vol 1, 2A & 2B, Bockris & Reddy, Plenum, New York, 2008.

5. Electrochemistry – Principles, Methods and Applications, Christopher M.A. Brett, Ana Maria and Oliveria Brett, Oxford University Press, Oxford & New York, 2007.

6. Electroanalytical Chemistry, B.H. Vassos and G.W. Ewing, John Wiley & Sons, New York, 2011.

7. Electrochemistry, S. Glasstone, EastWest Press, New Delhi, 2010.

MSC-402 C: SOLID STATE AND POLYMER CHEMISTRY **Marks: 30+70=100**
Total Credits: 4

Outcome: The course is directed at the application of solid and polymeric materials.

Course Outcome: Students will know the basic requirement within a solid and a polymeric material for different applications.

CO1: To give the knowledge of properties and application of solid.

CO2: To give the knowledge of classification of phase transition in solid.

CO3: To give the knowledge of mechanical behavior of polymers and thermodynamics of polymer solution.

CO4: To give the knowledge on thermodynamics of polymer solution.

CO5: To give the knowledge of structure property relationship and the stability of macromolecules.

Contents:

UNIT I: Electrical and magnetic properties of solids

Metals: calculation of density of states, origin of resistivity, weak paramagnetism. Semiconductors: intrinsic and extrinsic- p and n-types. Junctions and their applications - metal-metal, metal-semiconductor, semiconductor types and transistors.

Magnetic properties: classification of materials, cooperative phenomena, Magnetic domains, hysteresis.

Optical and dielectric properties of solids: piezo and inverse piezoelectric effects, ferroelectricity, ferroelectric transitions in $BaTiO_3$, photoconduction and photoelectric effects, photovoltaic effect, luminescence.

Superconductivity: Meisner effect, type I and type II superconductors, features of superconductors, Frolich diagram, Cooper pairs, theory of low temperature superconductivity, high temperature superconductivity. Applications of superconductors.

Unit II: Phase transition in Solids

Classification of phase transitions, first and second order phase transitions: Martensitic transition, order-disorder transitions and spinodal decomposition.

Unit III: Glass Transition Temperature

States of aggregation, states of phase, transitions and associated properties, factors influencing the Tg, Tg and molecular weight, Tg and plasticizers, Tg and melting point. Importance of Tg. Tg, Tm and Tf: Characteristics and evaluation of Tg, Tm and Tf in accordance with crystalline and amorphous polymers. Effect of temperature, crystallanity and molecular weight on mechanical behavior of polymers.

Unit IV: **Thermodynamics of Polymer Solutions**

Partial molar and partial specific quantities, chemical potential of macromolecular solution. Gibbs– Duhem equation, Polymer dissolution, thermodynamics of polymer dissolution, solubility of amorphous crystalline polymer, Flory-Huggins theory of polymer solutions, size and shape of macromolecules in solution.

Unit V: Mechanical Properties and Stability of Macromolecules

Mechanical properties: structure property relationship of polymers: strength, plastic deformation (rheology), physical state of polymers, chemical resistance, crystallanity, mechanism of deformation. Methods of testing: static testing, Poissons ratio, stress-strain curves. Transient testing and impact testing. Thermal degradation, oxidative and UV stability, chemical and hydrolytical stability, radiation effects. Mechanical degradation, photodegradation, degradation by ultrasonic waves.

Suggested Readings:

MSC-402 C: SOLID STATE AND POLYMER CHEMISTRY

Text Books/Reference Books:

1. Principles of the Solid State, H.V. Keer, Wiley Eastern Ltd., New Delhi, 1993.
2. Solid State Chemistry, D.K. Chakrabarty, New Age International Publishers, 2010.
3. Introduction to Solids, L.V. Azaroff, McGraw Hill Book Co., New York, 1960.
4. An Introduction to X-ray Crystallography, M.M. Woolfson, Cambridge University Press-Vikas Publishing House, New Delhi (1980).
5. Phase Transitions, C.N.R. Rao and K.J. Rao, Cambridge University Press
6. Solid State Chemistry and its applications. A. R West, John Wiley & Sons 2990
7. Text book of polymer science: F.W. Billmeyer (John.Wiley), London, 2010.
8. Polymer science: V.R. Gowariker, N.V. Viswanathan & T. Sreedhar (Wiley Eastern) New Delhi, 2011.
9. Introduction to Physical polymer science, L.H. Sperling, Wiley Interscience, New York, 2010.
10. Fundamentals of Polymer science and Engineering, Anil Kumar and S.K. Gupta, Tata McGraw hill LCUE Series, New Delhi, 2010.
11. Principles of polymer chemistry, P.J. Flory, Cornell Univeristy, Press Ithaca, 2012.

MSC-403: Physical Methods of Analysis **Marks: 30+70=100**

Total Credits: 4

***Outcome*: Students will be introduced to modern analytical techniques.**

***Course Outcome*: Students will be able to explain the application of different analytical techniques in chemistry.**

CO1: To give the knowledge of instrumentation and applications of X-ray diffraction technique and thermal methods towards the characterization of the solid.

CO2: To give the knowledge on the thermal methods of analysis of materials

CO2: To give the knowledge of surface study of solid catalyst.

CO3: To give the knowledge of high performance separation techniques.

CO4: To give the knowledge of different analytical spectroscopic methods.

Contents:

Unit I: Diffraction Techniques

Powder XRD and Single Crystal XRD: Technique, Instrumentation, Applications.

Unit II: Thermal Methods

Principles and applications of thermogravimetry analysis (TGA), Derivative thermogravimetry (DTG), Differential thermal analysis (DTA) and Differentail scanning calorimetry (DSC).

Unit III: Electron Microscopy

Scanning electron Microscopy (SEM) and Transmission Electron Microscopy (TEM): Technique, instrumentation and applications

Unit IV: Separation Techniques

GC, HPLC, GPC: Technique, instrumentation and applications

Unit V: Analytical Spectroscopic Methods

Atomic Absorption Spectroscopy (AAS)-theory, instrumentation and sampling

Atomic Emission Spectroscopy (AES)-theory, instrumentation and sampling. Applications of AAS and AES

Photoluminescence Spectroscopy (PL)-theory, instrumentation and applications

Photoelectron spectroscopy (UV and XPES): Principles and applications

Suggested Readings

MSC-403: Physical Methods of Analysis

Text Books/Reference Books:

1. D. B. Murphy, M. W. Davidson, Fundamentals of Light Microscopy and Electronic Imaging, Wiley, 2013.

2. D. B. Williams, C. B. Carter, Transmission Electron Microscopy A Textbook for Materials Science, Springer, 2009.

3. P. Eaton, P. West, Atomic Force Microscopy, Oxford University Press, 2010.

4. B. D. Cullity, Elements of X-Ray Diffraction, 3rdEdition, Addison Wesley Publishing Company, Inc., 2004.

5. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, B. Sivasankar, Vogel‘s Textbook of Quantitative Chemical Analysis,6th Edition, Pearson, 2009.

MSC 404: Project Dissertation **Marks: 60+140=200**

Total Credits: 8

Objective: **During the course, students are expected to learn different methods and techniques for carrying out scientific research problems, particularly to collect and interpret data.**

Students will also learn to survey research literature, and collect/compile the information for preparing reports and for publications.

Course Outcome: **Following the completion of this course, students should be able demonstrate ability to plan and strategize a scientific research problem, and implement it within a reasonable time-frame. It is expected that after completing this project dissertation, students will learn to work independently and how to keep accurate/readable record of their experimental work.**

In addition, students will be able to handle laboratory equipment and chemicals. Also, students will be able to utilize sophisticated instruments for analysis, data collection and interpretation.

Subsequently, the students should be able to critically examine research articles, and improve their scientific writing/communication skills.

CO1: To give the practical knowledge of multistep synthesis.

CO2: To give the practical knowledge of separation.

CO3: To give the practical knowledge of purification.

CO4: To give the practical knowledge of characterization by different spectroscopic techniques.

CO5: To give the knowledge of literature survey.

CO6: To give the knowledge of scientific writing.

CO7: To give the knowledge of use of software like chem. Draw, origin etc.

CO8: To give the knowledge of application and uses of synthesized compounds or materials.