

CURRICULUM

For

POSTGRADUATE DEGREE COURSE IN

BASIC SCIENCES
M.Sc. (CHEMISTRY)
(First Year)

[Proposed from 2018-19]



IIMT UNIVERSITY
MEERUT

IIMT University, Meerut

Study and Evaluation Scheme
Course: M.Sc. Chemistry
(Two Year Course)

Semester I

S.No.	Course Code	Subject	Periods			Credit	Evaluation Scheme		
			L	T	P		Internal	External	Total
1.	MSC-101	Inorganic Chemistry - I	4	1	-	4	30	70	100
2.	MSC-102	Organic Chemistry - I	4	1	-	4	30	70	100
3.	MSC-103	Physical Chemistry – I	4	1	-	4	30	70	100
4.	MSC-104	Computer for Chemists	4	1	-	4	30	70	100
5.	MSC-105	Mathematics for Chemists* OR Biology for Chemists*							50 Qualifying Only (40%)
6.	MSC-111P	Chemistry Lab – I (Inorganic, Organic, Physical Chemistry)	-	-	3	2	50	50	100
6.	ECC-111/112/113 /	Skill Enhancement	-	-		-	100	-	100
		Total	16	4	4	16	270	330	650

Study and Evaluation Scheme
Course: M.Sc. Chemistry
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Semester II

S. NO.	COURSE CODE	SUBJECT	EVALUATION SCHEME						
			L	T	P		INTERNAL	EXTERNAL	TOTAL
1.	MSC-201	INORGANIC CHEMISTRY - II	4	1	-	4	30	70	100
2.	MSC-202	ORGANIC CHEMISTRY - II	4	1	-	4	30	70	100
3.	MSC-203	PHYSICAL CHEMISTRY – II	4	1	-	4	30	70	100
4.	MSC-204	GROUP THEORY, SPECTROSCOPY & SOLID STATES	4	1	-	4	30	70	100
5.	MSC-211P	CHEMISTRY LAB – II(INORGANIC, ORGANIC, PHYSICAL CHEMISTRY)	-	-	3	2	50	50	100
6	ECC-211/212/213/214	SKILL ENHANCEMENT					100		100
		TOTAL	16	4	4	16	270	330	600

M.Sc. Chemistry I Year: I Semester
Inorganic Chemistry – I

Course Code MSC-101		L	T	P
		4	1	0

1. Stereochemistry and bonding in main group compounds **12 Hrs.**

VSEPR, Walsh diagrams (tri atomic molecules), $d\pi - P\pi$ bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

2. Metal – Ligand Equilibria in solution **8 Hrs.**

Stepwise and overall formation of constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH-metry and spectrophotometry.

3. Reaction Mechanism of Transition metal complexes **24 Hrs.**

Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories.

Kinetics of substitution reactions:- Acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without Metal-ligand bond cleavage. Substitution reaction in square planar complexes, the trans effect, mechanism of the substitution reaction.

Redox reactions (electron transfer reactions): Mechanism of one electron transfer reactions [such as Henry Taube's classical reaction of $(\text{NH}_3)_5\text{Co}^{3+}-\text{Cr}^{2+}$, Inner sphere type reactions]. Outer sphere type reactions (cross reactions) and Marcus hush theory (No mathematical treatment).

4. Metal Ligand bonding **16 Hrs.**

Adjusted CFT, limitations of crystal field theory. Octahedral, tetrahedral and square planar complexes.

Books Suggested:

1. Structural Inorganic Chemistry, A.F. Wells
2. Concise Inorganic Chemistry, J.D. Lee, Elbs with Chapman and Hall, London.
3. Theoretical Inorganic Chemistry, M.C. Day and J. Selbin, Reinhold, EWAP.
4. Elementary Coordination Chemistry, Jones
5. Coordination Chemistry, Martell
6. Organometallic Chemistry, T.S. Swain and D.S.T. Black.
7. Structure and Properties of Materials, Vol. 4, Electronic Properties, John Wulff, Wiley Eastern.
8. Advanced Inorganic Chemistry, F.A. Cotton and R.G. Wilkinson.
9. Atomic Structure and chemical Bonding, Manas Chanda.
10. Organometallic Chemistry, P.L. Pauson.

**M.Sc. Chemistry I Year: I Semester
Organic Chemistry – I**

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Course Code MSC-102		L	T	P
		4	1	0

1. Nature of bonding in organic molecules**10 Hrs.**

Delaocalised chemical bonding, Conjugation, hyper conjugation, bonding in fullerenes, tautomerism, Aromaticity in benzenoid and non benjenoid compounds, alternant and non-alternant hydrocarbons, Huckels's rule, energy levels of n molecular orbitals, annulenes, antiaromaticity, w-aromaticity, homo-aromaticity, PMO approach. Bond weaker than covalent – addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

2. Stereochemistry**15 Hrs.**

Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding. Elements of symmetry, chirality, molecules with more than one chiral center, thero and erythro isomers, methods of resolution, optical purity. Enantiotopic and diastereotopic atoms, groups and faces. Stereospecific and stereoselective synthesis; Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape. Stereochemistry of the compounds containing Nitrogen, Sulphur and Phosphorous.

3. Reaction mechanism: Structure and Reactivity**15 Hrs.**

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin – Hammet principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Hard and soft acids and bases. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes.

Effect of structure on reactivity – resonance and field effects, steric effects, quantitative treatment. The hammet equation and Linear free energy relationship, substituent and reaction constants, Taft equation.

4. Aliphatic Nucleophilic Substitution**15 Hrs**

Nucleophilic substitution at saturated carbon – SN1, SN2 and related mechanisms; Parameters influencing reaction rates; The Neighboring group mechanism, neighbouring group participation by π and σ bonds; Anchimeric assistance;

Classical and nonclassical carbocations, Phenonium ions, nonbornul system, common carbocation rearrangements, Application of NNMR spectroscopy in the detection of carbocations.

The SNi mechanism, Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium. Phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

5. Aliphatic Electrophilic Substitution**5 Hrs.**

Bimolecular mechanisms – SE2 and SE1. The SE1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Books Suggested:

1. Organic Chemistry, Vol. I & Vol. II, I.L. Finar, Longman.
2. Advanced Organic Chemistry, 2nd Edition, R.R. Carey and R.J. Sundberg.
3. Comprehensive Organic Chemistry, Barton and Ollis, Pergamon.
4. Organic Reactions, Various volumes, R. Adams.
5. Modern synthetic Reactions, H.O. House, Benjamin.

M.Sc. Chemistry I Year: I Semester
Physical Chemistry – I

Course Code MSC-103		L	T	P
		4	1	0

A. Thermodynamics**30 Hrs.****1. Classical Thermodynamics**

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar properties, partial molar free energy, partial molar volume and partial molar heat content and their significances. Determinations of these quantities. Concept of fugacity and determination of fugacity.

2. Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and micro canonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers).

Partition functions – translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions. Applications of partition functions.

Heat capacity behavior of solids – chemical equilibria and equilibrium constants in terms of partition functions, Fermi – Dirac statistics, distribution law and applications to metal. Bose Einstein statistics distribution law and application to helium.

3. Non Equilibrium Thermodynamics

Thermodynamic criteria for non equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the generalized fluxes and force, non equilibrium stationary states, phenomenological equations, microscopic reversibility.

B. Quantum chemistry**30 Hrs.****1. Introduction to Exact Quantum Mechanical Results**

The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

2. Approximate Methods

The variation theorem, linear variation principle, Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the Helium atom.

3. Angular Momentum

Ordinary angular momentum, generalized angular momentum, eigen functions for angular momentum, eigen values of angular momentum, operator using ladder operators. Addition of angular momenta, spin, anti symmetry and Pauli's exclusion principle.

4. Electronic Structure of Atoms

Electronic configuration, Russell – Saunders terms and coupling schemes, Slater – Condon parameters, term separation energies of the Pn configuration, term separation energies for the dn configurations, magnetic effects: spin – orbit coupling and Zeeman splitting, introduction to the methods of self consistent field, the virial theorem.

5. Molecular Orbital theory

Huckel theory of conjugated systems, bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc. Introduction to extended Huckel theory.

Books Suggested:

1. Advanced physical Chemistry, S. N. Blinder, The Macmilan Company.
2. Thermodynamics of Irreversible Processes, Ilya Prigogine.
3. Thermodynamics, R.C. Srivatsava, S. Saha and A.K. Jain, Prentice-Hall, India
4. Physical Chemistry, P.W. Atkins, ELBS.
5. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.
6. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum.
7. Modern Electrochemistry Vol. I & II, J.O.M. Bockris and A.K.N. Reddy, Plenum
8. Physical Chemistry (5th Ed.), I.N. Levine, Tata McGraw Hill Pub. Co. Ltd., New Delhi.
9. Introduction to Quantum Chemistry, AK Chandra, Tata McGraw Hill.
10. Quantum Chemistry, Ira N Levine, Prentice Hall.
11. Chemical Kinetics, K.J. Laidler, McGraw Hill.

M.Sc. Chemistry I Year: I Semester
Computers for Chemists

Course Code MSC-104		L	T	P
		4	1	0

This is a theory cum Laboratory course with more emphasis on laboratory work.

1. Introduction to Computers and Computing **8Hrs.**

Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/O devices. Secondary storage, Computer languages. Operating systems with DOS as an example. Introduction to UNIX and Windows. Data processing, principles of programming. Algorithms and flow-charts.

2. Computer Programming in FORTRAN/C/BASIC **12Hrs.**

The language features are listed here with reference to FORTRAN. The instructor may choose another language such as BASIC or C and the feature may be replaced appropriately. Elements of the computer language. Constants and variables. Operations and symbols. Expression. Arithmetic assignment statement input and output. Format statement. Termination statements. Branching statements such as IF or GO TO statement. LOGICAL variables, double Precision variables. Subscripted variables and DIMENSIONS. DO statements, FUNCTION and SUBROUTINE. COMMON and DATA statements.

Decision control structure, case control structure, functions, introduction on arrays, programmes based on above.

3. Programming in Chemistry **15 Hrs.**

Development of small computer course involving simple formula in chemistry such as Vander Waal's equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equation with in the Huckel Theory. Elementary structural features such as bond lengths, bond angles, dihedral angles etc. of molecule extracted from a data base such as Cambridge database.

4. Use of Computer Programmes **25Hrs.**

Execution of linear regression, X-V Plot, numerical integration and differentiation as well as differential equation solution programmes. Monte-Carlo and molecular dynamics. Introduction to MS Office (MS Word, MS Excel, MS Power Point). Lab sessions based on MS Office package, Introduction to Internet Explorer.

Books Suggested:

1. Computers and Common Sense, R. Hunt and J. Shelly, Prentice Hall.
2. Fortran 77, V. Rajaraman, Prentice Hall (India), New Delhi.
3. Computational Chemistry, A.C. Norris.
4. Schaum's Outline Series – Theory and Problems of Programming with Fortran Including structured Fortran, S. Lipschutz and A. Poe, McGraw Hill Book Company, Singapore.
5. Computers in Chemistry, K. V. Raman, Tata McGraw Hill (1993).

**M.Sc. Chemistry I Year: I Semester
Biology for Chemists**

Course Code MSC-105		L	T	P

1. Cell structure and Functions**5Hrs.**

Structure of prokaryotic and eukaryotic cells; Intracellular organelles and their functions; Comparison of plant and animal cells; Overview of metabolic process catabolism and anabolism; ATP – the biological energy currency.

2. Carbohydrates**8Hrs.**

Conformation of monosaccharide's; Structure and functions of important derivatives of monosaccharides like glycosides; Deoxy sugars, myoinositol, amino sugars; N acetylmuramic acid, sialic acid and disaccharides polysaccharides, Structural polysaccharides- cellulose and chitin; Storage polysaccharides - starch and glycogen; Ascorbic acid,

Carbohydrate metabolism: Kreb's cycle; Glycolysis, Glycogenesis and Glycogenolysis, Pentose phosphate pathway.

3. Lipids**6Hrs.**

Fatty acids, Essential fatty acids; Structures and function of triglycerides; Glycerophospholipids; Sphingolipids, Cholesterol, Bile acids, Prostaglandins; Lipoproteins composition and function; Properties of lipid aggregates– micelles, Bilayers, Liposomes and their possible biological functions; Biological members; Fluid mosaic model of membrane structure.

4. Amino acids, Peptides and Proteins**6Hrs.**

Chemical and enzymatic hydrolysis of proteins to peptides, Secondary structure of proteins, forces responsible for holding secondary structures. α -helix, β -sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein folding and domain structure, Quaternary structure.

Amino acid metabolism – degradation and biosynthesis of amino acids, sequence determination; chemical / enzymatic. Mass spectral, racemization/ detection.

5. Nucleic acids**5Hrs.**

Purine and Pyrimidine of nucleic acids and their synthesis; 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.

Books Suggested

1. Principles of Biochemistry, A.L.Lehninger, Worth Publishers.
2. Biochemistry, L.Stryer, W.H. Freeman.
3. Biochemistry, J. David Rawn, Neil Patterson.
4. Biochemistry, Voet and Voet, John Wiley.
5. Outlines of Biochemistry, E.E.Connand P.K.Stumpf, John Wiley.

**M.Sc. Chemistry I Year: I Semester
Mathematics for Chemists**

Course Code MSC-105		L	T	P

1. Vectors**5Hrs.**

Vectors, dot, cross and triple products etc. the gradient, divergence and curl vector calculus, Gauss' theorem, divergence theorem etc.

2. Matrix Algebra**5Hrs.**

Addition and multiplication, inverse, adjoint and transpose of matrices, special matrices (Symmetric, skew-symmetric, hermitian, skew-Hermitian, unit, diagonal, unitary etc.) and their properties. Matrix equations: Homogeneous, non – homogeneous linear equations and conditions for the solutions, linear dependence and independence.

Introduction to vector spaces, matrix eigenvalues and eigenvectors, diagonalization determinants (examples from Huckel theory).

Introduction to tensors; polarizability and magnetic susceptibility as examples.

3. Differential Calculus**10Hrs.**

Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc.) exact and inexact differentials with their applications to thermodynamic properties.

Integral calculus, basic rules for integration, integration by parts, partial fraction and substitution. Reduction formulae, applications of integral calculus.

Functions of several variables, partial differentiation, co-ordinate transformations (e.g. Cartesian to spherical polar), curve sketching.

4. Elementary Differential Equations**7 Hrs.**

Variable separable and exact first order differential equations, homogeneous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc., Solutions of differential equations by the power series method, Fourier series, solutions of harmonic oscillators and Legendre equation etc., spherical harmonics, second order differential equations and their solutions.

5. Permutation and Probability**3Hrs.**

Permutations and combinations, probability and probability theorems, probability curves, average, root mean square and most probable errors, examples from the kinetic theory of gases etc., curve fitting (including least squares fit etc.) with a general polynomial fit.

Books Suggested:

- 1.The Chemistry Mathematics Books, E. Steiner, Oxford University Press.
- 2.Mathematics for Chemistry, Doggett and Sucliffe, Longman.
- 3.Mathematical preparation for Physical Chemistry, F. Daniels, McGraw Hill.
- 4.Chemical Mathematics, D. M. Hirst, Longman.
- 5.Applied Mathematics for Physical Chemistry, J. P. Barrant, Prentice Hall.
- 6.Basic Mathematics for Chemists, Tebbutt, Wiley.

M.Sc. Chemistry I Year: I Semester
Chemistry Lab – I

Course Code MSC-111P		L	T	P
		0	0	3

Inorganic Chemistry

1. To analyse the mixtures of two components.
2. To analyse the mixture of three components.
3. To prepare Hexa-ammine (II) chloride
4. To Prepare Potassium dioxolatoCuprate (II) dehydrate
5. To prepare Potassium Trioxolato Chromate (III)
6. To prepare Tetra ammine Cupric sulphate
7. T prepare sodium ferric oxalate
8. To prepare crystals of PotasssiumTris Oxalate laminate (III)

Organic Chemistry

1. To identify the given organic compound and prepare its derivative.
2. To analyse the give organic mixture (water Separation).
3. Single step preparations:
 - a. Hydrolysis
 - b. Bromination
 - c. Nitration
 - d. Oxime formation
 - e. Reduction
 - f. Hoffmann Bromide reaction
 - g. Benzoin Condensation reaction

Physical Chemistry

1. To find out the strength of the given HCl solution by titrating it against N/10 NaOH using pH meter.
2. To find out the strength of the given CH₃COOH solution ny titrating it against N/10 NaOH using pH meter.
3. To find out the strength of HCl and CH₃COOH in a mixture of both by titrating it against N/10 NaOH using pH meter.
4. To determine the solubility of a give salt at room temperature and also draw its solubility curve.
5. To find out the heat of solution of oxalic acid by solubility method.
6. To standardize the give KMnO₄ solution by titrating it against Standard Ferrous Ammonium Sulphate solution.
- 7.

Books Suggested:

1. Vogel's Qualitative Inorganic Analysis, revised, svehla, Orient Longman.
2. Vogel's Textbook of Quantitative Inorganic Analysis (revised), J. Bassett, R.C. Denney, G.H. Jeffery and J. Mendham, ELBS.
3. Experimental Inorganic Chemistry, W.G. Palmer, Cambridge.
4. Laboratory Manuel in Organic Chemistry, R.K. Bansal, Wiley Eastern.
5. Experiments in General Chemistry, C.N.R. Rao and U.C. Agarwal, East-West Press.
6. Experiments in Physical Chemistry, R.C. Dass and D. Behra, Tata McGraw Hill.
7. Experiments in Physical Chemistry, J.C. Ghosh, BhartiBhavan.
8. Practical Organic Chemistry, F.G. Mann and B.C. Saunders, Pearson Education.

**M.Sc. Chemistry I Year: II Semester
Inorganic Chemistry – II**

Course Code MSC-201		L	T	P
		4	1	0

1. Electronic Spectra and Magnetic Transition Metal Complexes

22Hrs.

Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d1-d9 states), calculations of Dq , B and β parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

2. Metal π Complexes

18Hrs.

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls, preparation, bonding. Structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes, tertiary phosphine as Ligand.

3. Metal clusters

12Hrs.

Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

4. Nuclear Chemistry

8Hrs.

Radioactive decay & equilibrium. Nuclear Reactions, Q-value cross-sections, types of reactions, Chemical effects of nuclear transformations. Fission & Fusion, Fission products & Fission yields. Radioactive techniques, tracer techniques.

Books Suggested:

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes and Row.
3. Chemistry of the Elements, N.N. Greenwood and A. Earnshaw, pergamon.
4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Magnetochemistry, R.L. Carlin, Springer Verlag.
6. Comprehensive Coordination Chemistry, Eds. G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.

M.Sc. Chemistry I Year: II Semester
Organic Chemistry – II

Course Code MSC-202		L	T	P
		4	1	0

1. Aromatic Electrophilic Substitution**6 Hrs.**

The arenium ion mechanism, orientation and reactivity, energy profile diagrams, The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeier reaction, Gattermann-Koch reaction.

2. Aromatic Nucleophilic Substitution**5 Hrs.**

The S_NAr, S_N1, benzyne and S_{RN}1 mechanisms. Reactivity - effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles Rearrangements,

3. Free Radical Reaction**8 hrs.**

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenations (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction

4. Addition to Carbon – Carbon Multiple Bonds**6 Hrs.**

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration, Michael reaction, Sharpless asymmetric epoxidation.

5. Addition to Carbon – Hetero Multiple Bonds**12 Hrs.**

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids esters and nitriles, Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction.

Mechanism of condensation reactions involving enolates - Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

6. Elimination Reactions**5 Hrs.**

The E₂, E₁ and E_{1c}B mechanisms and their spectrum. Orientation of the double bond. Reactivity - effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

7. Pericyclic reactions**18 Hrs.**

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions- conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions- antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheletropic reactions.

Sigmatropic rearrangement, - Suprafacial and antarafacial shifts of H, Sigmatropic shifts involving carbon moieties, 3,3- and 5,5- Sigmatropic rearrangements. Claisen, Cope, Sommelet Hauser Rearrangement, Ene reaction.

Books Suggested:

1. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Orient longman.
2. Organic Reaction Mechanism, R. Breslow, Benjamin.
3. Mechanism and Structure in Organic Chemistry, B.S. Gould, (Holt Reinh).
4. Organic Chemistry, Hendrikson, Cram and Hammond, McGraw Hill.
5. Basic Principles of Organic Chemistry, J.D. Roberts and M.C. Caserio, Benjamin.
6. Organic Reaction Mechanism, R.K. Bansal, McGraw Hill.
7. Organic Chemistry, R.T. Morrison and R.N. Boyd, Prentice Hall.
8. Principle of Organic Synthesis, R.O.C. Norman and J.M. Coxon, ELBS.
9. Reaction Mechanism in Organic Chemistry, S.M. Mukharji and S.P. Singh.
10. Stereochemistry of Organic Compounds, D. Nasipuri.

11. Advanced Organic Chemistry, J. March, McGraw Hill.
12. Stereochemistry, P.S. Kalsi, New Age International.

M.Sc. Chemistry I Year: II Semester
Physical Chemistry – II

Course Code MSC-203		L	T	P
		4	1	0

1. Chemical Dynamics**20 Hrs.**

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions.

Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and oscillatory reactions (Belousov-Zhabotinsky reaction), homogeneous catalysis, kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method; relaxation method, flash photolysis and the nuclear magnetic resonance method. Dynamics of molecular motions, probing the transition state, dynamics of unimolecular reactions (Lindemann Hinshelwood and Rice-Ramsperger - Kassel- Marcus[RRKM] theories of unimolecular reactions.

20 Hrs.**2. Surface Chemistry****Adsorption:**

Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), Elementary treatment of BET Equation, catalytic activity at surfaces

Micelles:

Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization, solubilization, micro emulsion, reverse micelles.

Macromolecules:

Polymer-definition, types of polymers, kinetics of radical polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination (Elementary treatment of Osmometry, Viscometry, Sedimentation and Light scattering methods), chain configuration of macromolecules, calculation of average dimensions of various chain structures.

3. Electrochemistry**20 Hrs.**

Electrochemistry of solutions. Debye-Huckel - Onsager treatment and its extension, ion solvent interactions. Debye-Huckel-Jerum mode. Thermodynamics of electrified interface equations. Derivation of electro-capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Guoy-Chapman, Stern.

Over potentials, exchange current density, derivation of Butler Volmer equation, Tafel plot. Quantum aspects of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling, Semiconductor interfaces-theory of double layer at Semiconductor, electrolyte solution interface, structure of double layer interfaces. Electrocatalysis: influence of various parameters. Hydrogen electrode. Bio-electrochemistry, Polarography theory, Ilkovic equation, half wave potential and its significance.

Introduction of corrosion, homogenous theory, forms of corrosion, corrosion monitoring and prevention methods.

Books Suggested:

1. Advanced physical Chemistry, S. N. Blinder, The Macmillan Company.
2. Thermodynamics of Irreversible Processes, Ilya Prigofine.
3. Thermodynamics, R.C. Srivatsava, S. Saha and A.K. Jain, Prentice-Hall, India
4. Physical Chemistry, P.W. Atkins, ELBS.
5. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.
6. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum.
7. Modern Electrochemistry Vol. I & II, J.O.M. Bockris and A.K.N. Reddy, Plenum
8. Physical Chemistry (5th Ed.), I.N. Levine, Tata McGraw Hill Pub. Co. Ltd., New Delhi.

M.Sc. Chemistry I Year: II Semester
Group Theory, Spectroscopy and Solid State

Course Code MSC-204		L	T	P
		4	1	0

1. Symmetry and Group Theory in Chemistry

11 Hrs.

Symmetry elements and symmetry operation, definitions of group, subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies. symbols representations of groups by matrices (representaion for the C_n , C_{nc} , D_{nh} , D_{nh} etc. groups to be worked out explicitly). Character of a representation. The great orhtogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy.

2. Unifying principles

5 Hrs.

Electromagnetic radiation, interaction of electromagnetic radiation with matter: absorption, emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainty relation and natural line width, and natural line broadening. transition probability, results of time dependent perturbation theory, transition moment, selection rules, intensity of spectral lines, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels.

12 Hrs.

3. Vibrational spectroscopy

a. Infrared Spectroscopy

Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy. Breakdown of Oppenheimer approximation; vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal-ligand vibrations, normal co-ordinate analysis.

b. Raman spectroscopy

Classical and quantum theories of Raman effect. Pure rotational, vibrational and Vibrational-rotational Raman Spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti stokes Raman Spectroscopy (CARS).

4. Electronic spectroscopy

10 Hrs.

a. Atomic spectroscopy

Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

b. Molecular Spectroscopy

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

c. Photoelectron spectroscopy

Basic principles, photo-electric effect, ionization process, Koopman's theorem, Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA. Auger electron spectroscopy: basic idea.

5. Magnetic Resonance Spectroscopy

10 Hrs.

a. Nuclear Magnetic Resonance Spectroscopy

Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurements, factors influencing chemical shift, deshielding, spin-spin interactions, factors influencing coupling constant 'J'. Classification (ABX, AMX, ABC, A2B2 etc.), spin decoupling, basic ideas about instrument, NMR studies of nuclei other than proton-13C

b. Electron Spin Resonance Spectroscopy

Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications.

6. X-ray Diffraction

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

Books Suggested:

1. Chemical Applications of Group Theory, F.A. Cotton.
2. Modern Spectroscopy, J.M. Hollas, John Wiley.
3. Applied Electron Spectroscopy for Chemical Analysis, Ed. H. Windawi and F.L. Ho, Wiley Interscience.
4. NMR, NQE, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
5. Instrumental Methods of Analysis, Willard, Merrit, Dean and Settle.
6. Spectroscopic Identification of Organic Compounds, R.M. Silverstein and G.C. Bassler.
7. Spectroscopic Methods in Organic Chemistry, D.H. Williams and I. Fleming.
8. Absorption Spectroscopy of Organic Molecules, V.M. Parikh.
9. Applications of Spectroscopic Techniques in Organic Chemistry, P.S. Kalsi.
10. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
11. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
12. Theory and Applications of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH Oxford.
13. Introduction to Photo Electron Spectroscopy, P.K. Ghosh, John Wiley.
14. Introduction to Magnetic Resonance, A. Carrington and A.D. MacLachalan, Harper and Row.

**M.Sc. Chemistry I Year: II Semester
Chemistry Lab – II**

Course Code MSC-211P		L	T	P
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Inorganic Practical

1. Acidimetry – alkalimetry titration.
2. Oxidation reduction titration.
3. Complexometric – EDTA titration.
4. pH-metric titration.
5. Precipitation titration.
6. To estimate iron and nickel in a given solution.
7. To estimate copper and nickel in the given solution.

Organic Practical

1. Analysis of binary organic mixtures
 - a. Separation with NaHCO_3
 - b. Separation with NaOH
 - c. Separation with HCl
2. Two steps preparations:
 - a. To prepare anthranilic acid from phthalic anhydride.
 - b. To prepare o-chlorobenzoic acid from phthalamide.
 - c. To prepare benzyl from Benzaldehyde.
 - d. To prepare benzanilide from Benzophenone.

Physical Practical

1. To determine the relative strengths of two acids i.e., HCl and H_2SO_4 by studying the hydrolysis of methyl acetate.
2. To find out the rate constant of the hydrolysis of methyl acetate catalysed by (i) HCl and (ii) H_2SO_4 .
3. To find out the strength of HCl solution by titrating it against $\text{N}/10$ NaOH using conductometer.
4. To find out the strength of given NH_4OH solution by titrating it against HCl solution using Conductometer.
5. To determine the parachor value of given liquid.
6. To find out the surface tension of CH_3COOH , $\text{C}_2\text{H}_5\text{OH}$, n-Hexane at room temperature and hence calculate the atomic parachors of C, H and O.
7. To find out the surface tension of the given liquid by drop weight method at room temperature.

Books Suggested:

9. Vogel's Qualitative Inorganic Analysis, revised, vsehla, Orient Longman.
10. Vogel's Textbook of Quantitative Inorganic Analysis (revised), J. Bassett, R.C. Denney, G.H. Jeffery and J. Mendham, ELBS.
11. Standard Methods of Chemical Analysis, W.W. Scott, The Technical Press.
12. Experimental Inorganic Chemistry, W.G. Palmer, Cambridge.
13. Experimental Organic Chemistry Vol. I & II, P.R. Singh, D.S. Gupta and K.S. Bajpai. Tata McGraw Hill.
14. Laboratory Manuel in Organic Chemistry, R.K. Bansal, Wiley Eastern.
15. Experiments in General Chemistry, C.N.R. Rao and U.C. Agarwal, East-West Press.
16. Experiments in Physical Chemistry, R.C. Dass and D. Behra, Tata McGraw Hill.
17. Experiments in Physical Chemistry, J.C. Ghosh, Bharti Bhavan.
18. Practical Organic Chemistry, F.G. Mann and B.C. Saunders, Pearson Education.