

शहीद नंदकुमार पटेल विश्वविद्यालय, गढ़ उमरिया, ओड़िशा रोड, रायगढ़

SEMESTER SYLLABUS
M.Sc. CHEMISTRY

SCHEME OF EXAMINATION & DISTRIBUTION OF MARKS

SEMESTER - I

Paper No.	Title of the Paper (s)	Internal Assessment	Term End Exam	Practical	Total Marks
1.	Inorganic Chemistry	20	80		100
2.	Organic Chemistry, Stereochemistry & Pericyclic Reaction	20	80		100
3.	Physical Chemistry- I	20	80		100
4.	Spectroscopy And Mathematics/Biology For Chemists	20	80		100
LAB-I	Organic Chemistry				100
LAB-II	Analytical Chemistry				100
TOTAL					600

SEMESTER - II

Paper No.	Title of the Paper (s)	Internal Assessment	Term End Exam	Practical	Total Marks
1.	Inorganic Chemistry	20	80		100
2.	Organic Chemistry	20	80		100
3.	Physical Chemistry	20	80		100
4.	Spectroscopy, Diffraction Methods & Computer For Chemists	20	80		100
LAB-I	Inorganic Chemistry				100
LAB-II	Physical Chemistry				100
TOTAL					600

SEMESTER - III

Paper No.	Title of the Paper (s)	Internal Assessment	Term End Exam	Practical	Total Marks
COMPULSORY FOR GROUP A, B & C					
1.	Applications Of Spectroscopy	20	80		100
2.	Chemistry Of Bio-Inorganic & Bio-Organic	20	80		100
LAB-I	General (Compulsory)			200	200
OPTIONAL GROUP-A INORGANIC					
3.	Organotransition Metal Chemistry	20	80		100
4.	Photo inorganic Chemistry	20	80		100
OPTIONAL GROUP- B ORGANIC					
3.	Physical Organic Chemistry	20	80		100
4.	Chemistry Of Heterocyclic Compounds	20	80		100
OPTIONAL GROUP-C PHYSICAL					
3.	Chemistry Of Materials	20	80		100
4.	Advanced Quantum Chemistry	20	80		100
TOTAL					600

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SEMESTER SYLLABUS
M.Sc. CHEMISTRY

SEMESTER - IV

Paper No.	Title of the Paper (s)	Internal Assessment	Term End Exam	Practical	Total Marks
COMPULSORY FOR GROUP A, B & C					
1.	Photochemistry & Solid State Chemistry	20	80		100
2.	Bio-Physical & Environmental Chemistry	20	80		100
OPTIONAL GROUP-A INORGANIC					
3.	Bioinorganic Chemistry & Supra-Molecular Chemistry	20	80		100
4.	Analytical Chemistry	20	80		100
LAB-I	Special			200	200
OPTIONAL GROUP-B ORGANIC					
3.	Medicinal Chemistry	20	80		100
4.	Chemistry Of Natural Product	20	80		100
LAB-II	Special			200	200
OPTIONAL GROUP-C PHYSICAL					
3.	Liquid States	20	80		100
4.	Computation Chemistry	20	80		100
LAB-III	Special			200	200
				TOTAL	600
				GRAND TOTAL	2400

SEMESTER I
PAPER – I
INORGANIC CHEMISTRY

UNIT-I

Stereochemistry and Bonding in Main group Compounds – VSEPR theory, Walsh Diagram (Tri and Pentatomic Molecules) δ and π bonds, bent rule and energetic of hybridisation, some simple reaction of covalently bonded, molecules.

UNIT-II

Metal Ligand Bonding – Limitation of Crystal field Theory, Molecular orbital theory, octahedral, Tetrahedral and square planar complexes, π Bonding & molecular orbital theory.

UNIT-III

Electronic spectra of transition metal complexes – Energy levels in an atom, coupling of orbital angular momentum, determination of ground state term, derivation of term symbols. Electronic spectra of Transition metal complexes, Orgel and Tanabe- sugano-diagrams for Transition metal complexes.

UNIT-IV

- Magnetic Properties of transition metal complexes- Anomalous magnetic moment, Magnetic Exchange coupling and spin crossover, charge transfer spectra.
- Symmetry and Matrix representation- Symmetry Element & Symmetry operation, point Symmetry Group, schoenflies symbols, Matrix Representation of Symmetry Operations, Multiplication Table.

UNIT-V

Group Theory in Chemistry- Definition of group subgroup, relation between orders of a finite group and its sub group. Conjugate relation and classes, reducible & irreducible representations (Representation for C_n , C_{nv} , C_{nh} , D_{nv} , D_{nh} etc. Groups to be worked out-explicitly)

Books Suggested-

- Group Theory - Bhattacharya
- Advance Inorganic Chemistry – F.A. Cotton and Wilkinson: John Wiley.
- Inorganic Chemistry – J.E. Huhey Harpes & Raw
- Chemistry of the elements – N.N. Greenwood & A Earnshaw Pergamon.
- Inorganic Electronic Spectroscopy – A.B.P. Lever, Elsevier.
- Magneto Chemistry – R.L. Carlin Springer Verlag.
- Comprehensive Co-ordination Chemistry, G. Wilkinson R.D. Gillar's and J.A. McCleverty Pergamon.
- Chemistry Applications of Group Theory – F.A. Cotton.

SEMESTER-I

PAPER - II

ORGANIC CHEMISTRY, STEREOCHEMISTRY & PERICYCLIC REACTION

UNIT-I

Reaction Intermediates: Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes, nitrenes, and benzyne. Application of NMR in detection of carbocations.

Nature of Bonding in Organic Molecules: Delocalized chemical bonding, conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism. Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of π molecular orbitals, annulenes, homoaromaticity, PMO approach.

UNIT-II

Stereochemistry: 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 centre, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereo selective synthesis. Asymmetric synthesis, optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes). Chirality due to helical shape. Stereo chemistry of the compound containing nitrogen, sulphur and phosphorus.

UNIT-III

Reaction Mechanism: Structure and Reactivity: Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate. Potential energy diagrams, transition states and intermediates, methods of determining mechanism, isotope effects. Hammett equation and linear free energy relationship; substituent and reaction constants.

UNIT-IV

Pericyclic Reactions: Molecular orbital symmetry, frontier orbitals of ethylene 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams, FMO and PMO approach. Electrocyclic reactions, Conrotatory and disrotatory motions, $4n$, $4n+2$ and allyl systems. Cycloadditions - antarafacial and suprafacial additions, $4n$, $4n+2$ systems; $2+2$ addition of ketenes, 1,3 dipolar cyclo additions and cheletropic reactions. Sigmatropic rearrangements - Suprafacial and antarafacial shifts of H. sigmatropic shifts involving carbon moieties 3,3 and 5,5- Sigmatropic rearrangements, Claisen, Cope and Aza-Cope rearrangements. Fluxional tautomerism, Ene reaction.

UNIT-V

Molecular rearrangement: General mechanistic approach to molecular rearrangement reactions, carbocation rearrangement- migratory aptitude and memory effects. Brief study of following rearrangement reactions. Favoroskii, Baeyer-Villiger oxidation, Stork enamine reaction, Shapiro reaction, Sommelet rearrangement, Wittig's rearrangement, Grovenstein-Zimmerman rearrangement.

Books Suggested:

1. Advanced Organic Chemistry - Reaction Mechanism and Structure, Jerry March, John Wiley.

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SEMESTER SYLLABUS

M.Sc. CHEMISTRY

2. Advanced Organic Chemistry - F.A. Carey and R.K. Sundberg, Plenum.
3. A Guide Book to Mechanism in Organic Chemistry- Peter Syke longman.
4. Structure and Mechanism in organic chemistry - C.K. Ingold, Cornell University Press.
5. Organic Chemistry - R.T. Morrison and R.N. Boyd Prentice - Hall.
6. Modern Organic Reactions - H.O. House, Benzamic.
7. Principles of Organic Synthesis - R.P.C. Norman and J.M. Coxon, Blackie Academic and Professional.
8. Pericyclic Reaction - S.M. Mukherji.
9. Reaction Mechanism in Organic Chemistry - S.M. Mukherji and S.P. Singh Macmilan.
10. Stereochemistry of Organic compounds - D. Nasipuri New age International.
11. Stereochemistry of Organic Compounds - P.S. Kalsi, New Age International.

SEMESTER- I

PAPER - III

PHYSICAL CHEMISTRY-I

UNIT- I Quantum Chemistry:

Introduction in Exact Quantum Mechanical Result: The Schrodinger equation and the postulates of quantum mechanics. Discussion of solution of the Schrodinger equation to some model systems, viz. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

Approximate methods: The various theorems, linear variation principle. Perturbation theory (first order and non – degenerate). Application of variation method and perturbation theory to the Helium atom.

Angular Momentum: Ordinary angular momentum, generalized angular momentum, Eigen-functions for angular momentum, Eigenvalue of angular momentum; operator using ladder operators, addition of angular momenta, spin anti-symmetry and Pauli Exclusion Principle.

UNIT- II Atomic Chemistry:

Electronic Structure of Atoms: Electronic configuration, Russell – Saunders term and coupling scheme. Slater – Condon parameters, term separation energies of p^n configuration, term separation energies for d^n configurations, magnetic effects: spin – orbital coupling and Zeeman splitting, introduction to the method of self- consistent field, the virial theorem.

Molecular Orbital Theory: Huckel theory conjugated system, bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc. introduction to extended Huckel theory.

UNIT- III Chemical Dynamics:

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 nuclear magnetic resonance method, Dynamics of molecular motions, probing the transition state, dynamics of barrier less chemical reactions in solution, dynamics of unimolecular reactions (Lindemann-Hinshelwood and Rice- Ramsperger-Kassel-Marcus [RRKM] theories of unimolecular reactions).

UNIT- IV Surface Chemistry:

Adsorption: Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Calvin equation), and Gibbs adsorption isotherm, estimation of surface area (BET equation), surface film on liquids (Electro-Kinetic phenomenon), catalytic activity of surfaces.

Micelles: Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factor affecting the CMC of surfactants, counter ions binding to micelles, thermodynamics of micellization – phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

UNIT- V

Macromolecules: Polymer- definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetic of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering method), sedimentation, chain configuration of macro molecules, calculation of various chain structures.

Books Suggested:

1. Physical Chemistry; P. W. Atkins, ELBS.
2. Introduction to Quantum Chemistry; A. K. Chandra, Tata McGraw Hill.
3. Quantum Chemistry; Ira. N. Levine, Prentice Hall.
4. Coulson's Valence; R. Mc Weeny, ELBS.
5. Micelles Theoretical and Applied Aspects; V. Moroi, Plenum.
6. Introduction to Polymer Science; V. R. Gowarikar, N. V. Vishwanathan and J. Sridhar, Wiley Eastern.
7. Physical Chemistry of Surface; A. W. Anderson and A. Gast, Wiley.
8. Surfaces; G. Attard and C. Barnes, Oxford Univ. press.
9. Introduction to Solid state physics. Kittel, Wiley.
10. Crystal structure determination; W. Clegg, Oxford University Press.

SEMESTER I

PAPER – IV

SPECTROSCOPY AND MATHEMATICS/BIOLOGY FOR CHEMISTS

SECTION- A

UNIT- I

spectroscopy

Unifying Principles: 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 the time dependent perturbation theory, transition moment. Selection rules, intensity of spectral lines. Born-Oppenheimer approximation, Rotational, Vibrational and Electronic Energy Levels.

UNIT- II

Microwave Spectroscopy: Classification of Molecules, rigid rotor model effect of isotopic substitution on the transition frequencies, Intensities, non-rigid rotor. Stark effect, Nuclear and Electron spin Interaction.

Raman Spectroscopy: Classical & Quantum Theories of Raman Effect. Pure rotational, vibrational & vibrational rotational Raman Spectra, Selection rules, Mutual exclusion Principle, Resonance Raman Spectroscopy, Coherent, Antistokes, Raman Spectroscopy (CARS).

UNIT- III

Vibrational Spectroscopy: 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, vibrational, rotation spectroscopy. P.Q.R. branches. Breakdown of oppenheimer approximation. Vibration of poly atomic molecules. Selection rules, normal modes of vibration, group frequencies overtones hot bands factors affecting the band positions and intensities for IR region.

SECTION- B

MATHEMATICS FOR CHEMISTS

(For Students without Mathematics in B.Sc.)

UNIT- IV

Vector and Matrix Algebra

Vectors: - Vector dot, cross and triple products etc. The gradient divergence and curl. Vector calculus, gauss Theorem divergence Theorem etc.

Matrix Algebra: - Addition and Multiplication, Inverse, adjoint and transpose of matrices. Special matrices. (Symmetric, Skew symmetric, diagonal, unitary etc.) And their properties, matrix equation, Homogeneous, Non Homogeneous linear equations.

Differential Calculus: Functions, continuity and differentiability rules for differentiation, Applications of differential calculus. Including maxima and minima. Exact & Inexact differentials with their Application to thermodynamics properties. Integral calculus, basic Rules for Integration, Integration by parts, partial fraction and substitution. Reduction formulae, Applications of integral calculus. Functions of several variables.

UNIT- V

Elementary differential equations: Variables-Separable and Exact First-order, differential equation, homogeneous, Exact and linear equation. Applications to Chemical Kinetics, Secular Equilibrium quantum chemistry.

Permutation and Probability: Permutations and combinations, probability and probability theorem, probability curves, average, root mean square and most probable errors, examples from kinetic theory of gases.

OR
SECTION- B
BIOLOGY FOR CHEMISTS
(For Student without Biology In B.Sc.)

UNIT- IV

Cell Structure and Functions: Structure of prokaryotic and eukaryotic cells-Intercellular organelles and their functions. Comparison of Plant and animal cells. Overview of metabolic processes- catabolism and anabolism. ATP- The biological Energy currency. Origin of life - unique properties of carbon. Chemical evolution and rise of living systems. Introduction to bio molecules, building blocks of Bio-macromolecules.

Carbohydrates: Conformation of mono-saccharides, structure and function of important derivatives of monosaccharide. Like glycosides-deoxy sugar myoinositol, Aminosugar, disaccharides and polysaccharides structural. Poly saccharides cellulose and chitin. Storage polysaccharides starch and glycogen. Carbohydrate of glyco-protein and glycolipids. Role of sugar in biological recognition. Blood group substances. Ascorbic Acid, Carbohydrate metabolism, Krebs cycle, Glycolysis, Glycogenesis and Glycogenolysis, Gluconeogenesis, pentose phosphate pathway.

UNIT- V

Lipids: Fatty acids, essential fatty acids, structure and function of triglycerals glycerophospholipids, Sphingolipids cholesterol, bile acids, prosta-glandins lipoproteins-composition and function role in atherosclerosis. Properties of lipid aggregates micelles bilayers. Liposomes and their possible biological functions, Biological membranes, fluid mosaic model of membrane spectra liquid metabolism. β -Oxidation of fatty acids.

Amino acids, Peptides and Proteins: Chemical & enzymatic hydrolysis of proteins to peptides, Amino Acid sequencing, secondary structure of proteins, forces responsible for holding of secondary structure., 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 acid. Sequence determination. Chemistry of Oxytocin and tryptophane releasing hormones (TRH)

Nucleic Acid: Purine, Pyrimidine, bases of Nucleic acid, base pairing, via H-bonding, structure of Ribo Nucleic Acid (RNA) & D.N.A. deoxy ribonucleic acid, double helix model of DNA and forces responsible for holding at chemical and Enzymatic Hydrolysis of Nucleic Acid. The Chemical bases of heredity, an overview of replication of DNA. Transcription, translation and genetic code, chemical synthesis of mono and Trinucleosides.

Book Suggested for Spectroscopy :

1. Modern Spectroscopy - J.M. Hollas Hohnwiley.
2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windowi and F.L. Ho Willey Interscience.
3. NMR, NQR, ESR and mossbaure spectroscopy in Inorganic chemistry :- R.V. Parish, Ellis Harwood.
4. Physical Method in Chemistry - R.S. Drago, Saunders College.
5. Introduction to Molecular Spectroscopy - G.M. Barrow, Mcgraw Hill.
6. Basic Principle of Spectroscopy- R. Chang Mcgraw Hill.
7. Theory and Application of Uv Spectroscopy H.H. Jaffe, and M. Orchin, IBH Oxford.
8. Introduction to Photo electron spectroscopy P.K. Ghosh John Wiley.

SEMESTER SYLLABUS
M.Sc. CHEMISTRY

9. Introduction to magnetic Resonance. A. Carrington and A.D. MacLachlan Harper & Row.

10. H. Kaur, Spectroscopy, Wiley.

Books: Mathematics for chemists:

1. The Chemistry Mathematics Book: E.Steiner, Oxford University Press.
2. Mathematics for Chemistry - Eggeff and Sectcliffe longman.
3. Mathematical preparation for physical chemistry - F. Daniels McGrow Hill.
4. Chemical Mathematics - D.M. Hirst- Longmann.
5. Applied Mathematics for Physical Chemistry - J.R. Barrato, Prentice Hall.
6. Basic Mathematics for Chemists Tebbutt Wiley.

Books -Biology for chemists

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 & Voet John Wiley.
5. Biochemistry, Jain & Jain, S. Chand.

SEMESTER I
LABORATORY COURSE - I
ORGANIC CHEMISTRY

1. Qualitative Analysis:-

Separation, Purification and Identification of compounds of Binary Mixture, T.L.C. and Column chromatography. I.R. Spectra may be used for functional group identification of compound by suitable derivatives preparation and determination of their melting points.

2. Organic Synthesis:-

1. Bromination - Preparation of p-Bromo Aniline from Acetanilide.
2. Nitration - Preparation of p-Nitro Aniline from Acetanilide
3. Hoffman Bromide Reaction. Preparation of Anthranilic Acid from Pthallic anhydride.
4. Aldol Condensation - Dibenzal acetone from Benzaldehyde.
5. Sandmeyer Reaction -
 - o-Chloro Benzoic Acid from Anthranilic Acid.
 - p- Chloro toluene from Toluene.
6. Friedal Craft Reaction - p-Benzoyl Propionic Acid from Succinic Anhydride and Benzene.
7. Oxidation - Adipic Acid by Chromic Acid oxidation of cyclohexanol.
7. Diazotization:-
 - Preparation of methyl orange from Sulphanilic Acid.
 - Phenyl Azo- Naphthol from Aniline.
8. Preparation of Acridone from N- Phenyl anthranilic acid.
9. Grignard's reaction: Synthesis of triphenylmethanol from Benzoic acid.

Note: Two stage preparation. Preparation of pure and crystalline compound based on any two of above principals with confirmation of melting point.

3. Quantitative Analysis:-

1. Determination of the percentage or number of Hydroxyl group in an organic compound by Acetylation method.
2. Estimation of Amines/Phenols using Bromate - Bromide Solution / or Acetylation method.
3. Determination of equivalent- weight of carboxylic compound.
4. Estimation of carboxyl group by titration / silver salt-method.
5. Estimation of Carbonyl group by Hydrazone method.
6. Estimation of Glycine by titration.

Instruction to Practical Examiners in Chemistry Semester – I

1. The Board of Examiners; one external and one internal for each branch will meet to decide the exercises and other matter in connection with the conduct of practical examinations

S. No.	Lab. Course (branch)	Max. Marks	Duration
1.	I- Organic Chemistry	100	5 hrs.
2.	II- Analytical Chemistry	100	5 hrs.

2. The distribution of marks is as under. Marks of Ex-students are given in parentheses.

(a) Qualitative Analysis of mixture containing two Organic compounds	30 (40) marks
(b) Preparation	10 (15) marks
(c) Estimation	20 (25) marks
(d) Viva voice	20 (20) marks
(c) Sessional	20 (-) marks

Total-100 (100) marks

As far as possible all the exercises as laid down in the syllabus are set. The scale of marking will be determined by examiners in accordance with the nature of exercises.

SEMESTER I
LABORATORY COURSE II
ANALYTICAL CHEMISTRY
SECTION- A

INSTRUMENTATION AND COMPUTERS

1. Error Analysis & Statistical data Analysis:-
Errors, types of errors, Minimization of Error, Statistical treatment for error analysis, standard deviation, Relative standard deviation, Linear least square. Calibration of volumetric apparatus burrettes pipette, standard flask, weight-box etc.
2. Volumetric Analysis:-
Basic Principles, determination of I_2 and saponification values of oil sample determination of DO, COD, BOD, Hardness of water samples.
3. Chromatography:-
Separation of Cations and anions by (A) Paper Chromatography, (B) Column Chromatography.

SECTION- B

4. pH Mety / Potentiometry / Conductometry titration :-
Determination of strength of acid etc.
5. Flame Photometry / AAS/FIA/Colorimetry :-
Determination of Cations / anions and metal ions eg. Na^+ , K^+ , Ca^{2+} , SO_4^{2-} , NO_2^- , Fe, Mo, Ni, Cu, Zn etc.
6. Spectro Photometry :-
Verification of Beer - Lambert Law. Molar Absorptivity calculation. Plotting graph to obtain λ_{max} etc. effect of pH in aqueous coloured system. Determination of metal ions eg. Fe, Cu, Zn, Pb etc
7. Nephelometry / Turbidimetry :- Determination of chlorine, sulphate phosphate turbidity etc.
8. Application of Computer in Chemistry:- As Specified in Theory paper in section II (A).

For Lab. Course -II (Analytical Chemistry):

(a) Two practical exercise (one from each section) (at least one of these will be based on instrumental analysis)	60 (80) marks
(b) Viva voice	20 (20) marks
(c) Sessional	20 (-) marks
	Total- 100 (100) marks

As far as possible all the exercises as laid down in the syllabus are set. The scale of marking will be determined by examiners in accordance with the nature of exercises. Sessional marks will be awarded by External Examiner in consultation with the internal Examiner