Deen Dayal Upadhyaya Gorakhpur University Gorakhpur



Two Year M.Sc. Degree Course in CHEMISTRY

CHOICE BASED CREDIT SYSTEM SYLLABUS

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1. Title of the Course: M.Sc. Chemistry

2. Preamble of the Syllabus:

Master of Science (M.Sc.) in Chemistry is a post graduation course of Deen Dayal Upadhyay Gorakhpur University, Gorakhpur. The aim of this programme is to impart indepth knowledge and skill to meet the current needs of industry, educational and R&D institutions. The revised curriculum is based on Choice based credit system and is developed with a viewpoint to keep pace with quality and quantity of knowledge of modern chemical science. In formulating these courses care has been taken to keep in mind the regional and national priorities maintain national and international educational standards.

The term credit is used to describe the quantum of syllabus for various programs in terms and hours of study. It indicates differential weightage given according to the contents and duration of the courses in the Curriculum design. Credit based system is flexible curriculum pattern with many merits. It is devoid of many limitations associated with the conventional rigid pattern of curriculum. Each course is assigned a weight (credit) depending upon its relative importance to the programme of definite total credit rating. In addition, several elective papers (choices) have been included in order to suit for the career of the students.

The curriculum to be implemented with this system would allow students to migrate between different institutions due to their own compulsions without losing their precious time. This system also has a benefit for students to develop a strong footing in the fundamentals with flexibility in selecting courses of specialization in the discipline of his/her liking and abilities.

3. Introduction

- **a.** Master's degree course in chemistry would be of 100 credits, where one credit course of theory will be of one clock hour per week running for 15 weeks and one credit of practical course will consist of two clock hour per week running for 15 weeks.
- **b.** Every student shall complete 100 credits in four semesters. All semesters will have 25 credits each.
- c. In each semester, there will be 4 theory papers of 4 credits each. Thus there will be 16 credits for theory papers in each semester. In each semester, practical course will be of 8 credits. 1 credit will be for seminar in each semester.
- **d.** Academic calendar showing dates of commencement and end of teaching and term end examination will be prepared and duly notified before commencement of each semester every year.

Ordinance for CBCS course is attached at the end of syllabus

4. Course Structure

The following are the papers in M.Sc. Chemistry course:

M.Sc. I Semester

Paper No.	Paper Name	No. of Units	Max. Marks	No. of Credits
CH-101	Molecular Symmetry and	05	100	04
(Core)	Molecular Vibrations			
CH-102 (Core)	Quantum Chemistry-I	05	100	04
CH-103 (Core)	Main Group Elements	05	100	04
CH-104 (Core)	Organic Reaction Mechanism	05	100	04
CH-105 (Core)	Practical		200	80
	Seminar		25	01

M.Sc. II Semester

Paper No.	Paper Name	No. of Units	Max. Marks	No. of Credits
CH-201	Analytical Chemistry	05	100	04
(Core)			200	0.1
CH-202	Thermodynamics and	05	100	04
(Core)	Electrochemistry			
CH-203	Transition Elements	05	100	04
(Core)				
CH-204	Natural Products	05	100	04
(Core)				
CH-205	Practical		200	08
(Core)				
	Seminar		25	01

M.Sc. III Semester

Paper No.	Paper Name	No. of	Max.	No. of
		Units	Marks	Credits
CH-301	Spectroscopy-I	05	100	04
(Core)				
CHP-302	Quantum Chemistry-II	05	100	04
CIII 202	Chamical Applications of Commentury	٥٢	100	0.4
CHI-302	Chemical Applications of Symmetry	05	100	04
	and Group Theory			
CH0-302	Stereochemistry	05	100	04
CHP-303	Electrodics and Electrochemical	05	100	04
	Phenomena			
CHI-303	Coordination Chemistry	05	100	04
CHO-303	Pericyclic and Rearrangement	05	100	04
	Reactions			
CHP-304	Thermodynamics and	05	100	04
	Intermolecular forces			
CHI-304	Supramolecular Chemistry	05	100	04
CHO-304	Biomolecules	05	100	04
CHP-305	Practical		200	08
CHI-305	Practical		200	08
CH0-305	Practical		200	08
	Seminar		25	01

- a. CH-301 is compulsory paper (core)
- b. All others are elective papers; students should opt either all papers from series CHP or from series CHI or from series CHO

M.Sc. IV Semester

Paper No.	Paper Name	No. of	Max.	No. of
		Units	Marks	Credits
CH-401	Spectroscopy-II	05	100	04
(Core)				
CHP-402	Chemical Kinetics, Solid State and	05	100	04
	Reaction Dynamics			
CHI-402	Bioinorganic Chemistry	05	100	04
CH0-402	Organic Synthesis	05	100	04
CHP-403	Statistical Mechanics	05	100	04
CHI-403	Organo Transition Metal Chemistry	05	100	04
CHO-403	Select Topics in Organic Chemistry	05	100	04
CHE-404	Polymer Chemistry	05	100	04
CHE-405	Inorganic Materials	05	100	04
CHE-406	Drugs and Agrochemicals	05	100	04
CHE-407	Solid State Chemistry	05	100	04
CHE-408	Nuclear and Radiation Chemistry	05	100	04
CHE-409	Biophysical Chemistry	05	100	04
CHE-410	Computational Chemistry	05	100	04
CHP-411	Practical		200	08
CHI-411	Practical		200	08
CHO-411	Practical		200	08
	Seminar		25	01

- a. CH-401 is compulsory paper (core)
- b. All others are elective papers; students should opt either all papers from series CHP or from series CHI or from series CHO and any one from series CHE

Semester-I

CH-101: Molecular Symmetry and Molecular Vibrations

(4 Credits) (60L)

Unit-1 (15 L)

Symmetry elements and symmetry operations with special reference to water and ethane.

Classification of molecules/ions based on their symmetry properties.

Unit-2 (18L)

Derivation of matrices for rotation, reflection, rotation-reflection and inversion operations, Symmetry point groups applied to all type of molecules (C_{nh} , D_{nh} , C_{nv} , T_d , O_h and I_h).

Unit-3 (10L)

Group multiplication basis, matrix representation, character of an operation, orthogonality, character tables, reducible and irreducible representations, groups, subgroups and classes.

Unit-4 (10L)

Symmetry of normal vibrations, determination of normal modes by internal and Cartesian coordinates methods, mixing of internal coordinates in normal modes, selection rules for IR and Raman spectroscopy.

Unit-5 (07 L)

Normal coordinate analysis of water and ammonia molecules and their infrared and Raman spectral activity.

Books Recommended:

- 1. D.M. Bishop, "Group theory and Chemistry" Dover Publications.
- 2. F.A. Cotton, "Chemical Applications of Group Theory", John Wiley, 1971.
- 3. M. Hamaresh, "Group theory and its Applications to Physical Problems" Addison-Wisley
- 4. McWeeny, "Symmetry An Introduction to Group Theory", Pergamon Press.
- 5. Lowell H. Hall "Group Theory and Symmetry in Chemistry", McGraw Hill Book Company, New York, 1969
- 6. K.VeeraReddy, "Symmetry and Spectroscopy of Molecules", New Age International Limited Publisher, New Delhi.

CH-102: Quantum Chemistry I

(4-Credits) (60L)

Unit-1 (15L)

Fundamental Concepts:

- **a.** Operators and algebra of operators, commutators, Linear operators, Vector operators, Laplacian operators, Hermitian operators, Concept of normalization and orthogonality in wave function.
- **b.** Postulates of quantum mechanics.
- **c.** Schrodinger equation and particle in one dimensional and three-dimensional box and degeneracy of states.

Unit-2 (15L)

Quantum mechanical treatment:

- a. Quantum mechanical treatment of a harmonic oscillator, One dimensional Harmonic oscillator (Classical and quantum mechanical treatments), Energy levels of harmonic and an-harmonic oscillators
- b. Quantum mechanical treatment of a rigid rotor
- c. Rigid rotor model of a diatomic molecule, Energy levels of a rigid rotor, Rigid rotor selection rule, A non rigid rotor.

Unit 3 (10L)

Schrodinger equation for H atom:

Transformation of coordinates, Separation of Variables, ϕ , θ and R equations and their solutions, Spherical harmonics, electron spin.

Unit 4 (10L)

Many - Electron Atoms:

Antisymmetry and Slater determinant for the wave function of ground state of multielectron atom, Self consistent field approximation (Hartree's Theory).

Unit 5 (10L)

Approximation methods:

The variation method, Perturbation method and First order Perturbation theory.

- 1. Quantum Chemistry by Donald A. Macquarrie
- 2. Molecular Quantum Mechanics by P.W. Atkins and R.S. Friedman
- 3. Quantum Chemistry by R. K. Prasad
- 4. Introductory Quantum Chemistry by A. K. Chandra
- 5. Quantum Chemistry by Ira N. Levine
- 6. Physical Chemistry by T. Engel and P. Reid

CH-103: Main Group Elements

(4 Credits) (60L)

Unit-1 (08L)

Stereochemistry of Bonding in Main Group Components:

 $d\pi$ – $p\pi$ bonds, Bents rule, Energetics of hybridization

Unit-2 (10L)

Preparation, Structure, Bonding and Technical Applications of,

- a. Polyether complexes of alkali and alkaline earth metals
- b. Polyphasphazenes
- c. Thiazyl and its polymers, tetrasulfur dinitride.

Unit-3 (08L)

- **a.** Structure and bonding of Borane anions
 - b. Classification and structures of Silicates

Unit-4 (08L)

Synthesis and structure of:

a. Carbides (05L)

b. Polyions of Ge, Sn, Pb, Sb, Bi and Hg (08L)

Unit-5

- a. Definition and classification of organometallic compounds on the basis of hapticity and polarity of metal-carbon bond (3L)
- b. Preparation, Properties, Structure and Applications of alkyl and aryls of Lithium,Beryllium, Aluminum, Mercury and Tin. (10L)

- 1. Advance Inorganic Chemistry, 6th Edition, Cotton and Wilkinson
- 2. Inorganic Chemistry, 4th Edition, Principles of Structure and Reactivity by J.F. Huheey, E.A. Keiter and R.L. Keiter, 1993
- 3. Chemistry of Elements by N.N. Greenwood and A. Ernshaw, Butterworths 1997
- 4. Organometallic Chemistry: A Unified Approach by R.C. Mehrotra and A.K. Singh
- 5. Comprehensive Coordination Chemistry Vol.3 by G. Wilkinson, R.D. Gillard, And J.A. McCleverty, Pergamon Press 1987.

CH-104: Organic Reaction Mechanism

(4 Credits) (60L)

Unit-1 (10L)

Basic principle of organic reaction mechanism:

Potential energy diagram ,transition state and intermediates, methods of determination of organic reaction mechanism, kinetic isotopic effect and its importance in determination of reaction mechanism.

Unit-2 (18L)

Substitution Reactions:

- a. **Aromatic electrophilic substitution:** General view, energy profile diagram, arenium ion mechanism (ArSE) of different aromatic electrophilic substitution reactions, ipso-substitution and ortho/para ratio.
- Aromatic nucleophilic substitution: (ArSN) Addition- elimination and elimination- addition (benzyne) mechanisms, effect of structure of substrate, nucleophile and leaving group on ArSN reaction.
- c. Aliphatic nucleophilic substitution: Mechanism and stereochemistry of $S_N{}^1$, $S_N{}^2$, $S_N{}^2$ and $S_N{}^i$ reactions, role of substrate's structure, nuleophiles, leaving group and solvent on SN reactions. Nuleophilic substitution at bridged head carbon atom.
- d. **Neighouring group participation (NPG):** Evidence for NGP, participation of sigma., Pi- bonds, halogen, N-atoms and phenyl ring.

Unit-3 (10L)

Elimination reaction:

 E_1 , E_2 and E_1 cb mechanisms, orientation (Saytzef's and Hoffmann eliminations), pyrolytic (syn) elimination, stereochemistry of E_2 reaction, factors affecting E_1 , E_2 and E_1 cb reactions, Competition between substitution and elimination reactions.

Unit-4 (10L)

C=C Bond Addition:

Mechanism and stereochemistry of addition of halogen and halogen acids to alkenes,1,2-hydroxylation, hydroboration, oxymercuration-demercuration , hydrogenation of alkynes, epoxidation, Corey epoxidation and cyclopropanation, Simmon-Smith cyclopropanation and Sharpless asymmetric epoxidation (SAE).

Unit-5 (12L)

C-Hetero multiple Bond addition:

Mechanism of hydrolysis of ester and amide. Crame's rule. Condensation reaction involving Cannizzaro, Claisen and Knovenagel.

- 1. Advanced Organic Chemistry Part. A & B By F. A. Carey and R. J. Sundberg, Plenum Publisher, New York, 2007.
- 2. Advanced Organic Chemistry By J. March, 2007.
- 3. Organic chemistry By J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxford University Press , New York, 2001.

Semester-I

Practical and Seminar

(8+1 Credits) (24h/week)

Marks (Practical): 200; Time: 12h in two days; Marks (Seminar): 25

Marks distribution (Practical)

Physical: 40

Inorganic: 40

Organic:40

Viva: 30

Record: 20

Internal Assessment: 30

Physical Chemistry exercises:

- 1. Determination of the solubility of benzoic acid in water at different temperatures and calculate the heat of solution
- 2. Determination of the distribution coefficient of benzoic acid between benzene and water
- 3. Determination of the distribution coefficient of acetic acid between benzene and water
- 4. Determination of the distribution coefficient of iodine between carbon tetrachloride and water
- 5. Study the adsorption of acetic acid on charcoal and draw the Freundlich isotherm
- 6. Conductivity measurement and conductometric titration of strong acid and strong base.

Inorganic Chemistry exercises:

Qualitative analysis of an inorganic mixture of seven radicals including Tl, W, Se, Te, V, Be, U, Ti, Zr, Th, Ce and Li, in addition to the radicals prescribed for the B.Sc. course. Semi-micro analysis is to be done

Organic Chemistry exercises:

Preparation of organic compounds involving two stages. Emphasis should be given in the following processes:

Purification, distillation under reduced pressure, steam distillation and fractional crystallization

Semester-II

CH-201: Analytical Chemistry

(4 Credits) (60L)

Unit-1 (20 L)

Electroanalytical Techniques:

- **a. Conductometric:** Discussion of the nature of the curves of acid-base (including mixtures of acids), precipitation and complexometric titrations
- **b. Potentiometric:** Different types of electrodes, discussion of the nature of the curves for oxidation-reduction and acid-base titrations, comparision with the conductometric method
- c. Voltametry: Cyclic voltametry
- **d. Polarography:** Dropping mercury electrode and its advantages, polarographically active species, concept of residual, diffusion and limiting current of half wave potential, Ilkovic equation and factors affecting diffusion current

Unit-2 (15L)

Thermoanalytical Methods:

- a. Thermogravimetry: Apparatus, factors affecting TG, Interpretation of TG curves of $CaC_2O_4.H_2O$ and $MgC_2O_4.2H_2O$
- **b. Differential Thermal Analysis and Differential Scanning Calorimetry:** Apparatus, factors affecting DTA and DSC curves with special reference to heating rate, particle size and packing, measurement of heat of transition, heat of reaction and heat of dehydration of salts and metal hydrates.

Unit-3 (09L)

Radiochemical Methods

- a. Isotope method
- b. Inverse isotopic dilution
- c. Neutron activation technique

Unit-4 (10L)

Chromatographic Method:

- a. **Gas Chromatography:** GLC and GSC
- b. HPLC

Unit-5 (6L)

Spectral Methods:

- a. Nephelometry
- b. Turbidimetry
- c. Flame Photometry

- 1. Fundamentals of Analytical Chemistry: D.A. Skoog, D.M. West and F.J. Holler, 1992, 6e
- 2. Quantitative Inorganic Analysis, A.I. Vogel, 2012, 7e
- 3. Instrumental Methods of Chemical Analysis: B.K. Sharma, 2011
- 4. Instrumental Methods of Chemical Analysis: H. Kaur, 2016, 12 e
- 5. Analytical Chemistry, Gary D. Christian, 2007, 6e
- 6. Instrumental Methods of Analysis: H.H. Willard, L.L. Merrit, Jr. J.A. Dean, 1974, 5e

CH-202: Thermodynamics and Electrochemistry

(4 Credits) (60L)

Unit 1 (20L)

a. Some important thermodynamic effects and relationships:

The Joule Thomson's effect, The Gibbs Helmoltz equation and its application, The ClausiusClapeyron equation, The Maxwell,s relation, Thermodynamics equation of state(Relationship between EorH and P,V,T).

b. Partial molar Properties

Partial molar quantities,(partial molar volume and partial molar Gibbs energy),Experimental determination of partial molar volume, Chemical potential and variation of chemical potential with temperature and pressure, The Gibbs Duhem equation

c. Fugacity and Activity

Fugacity, variation of fugacity with temperature and pressure, Activity and the activity coefficient, determination of activity and activity coefficients of non-electrolytes.

Unit 2 (09L)

The Third law Thermodynamics:

The third law, Nernst heat theorem, Calculation of entropy.entropy of real gases, application of third law, The residual entropy.

Unit 3 (08L)

Electrolytic Conductance of strong electrolytes:

Debye-Falkenhagen effects, Wein effects the ionic association, effect of ionic strength on rate of ionic reactions.

Unit 4 (08L)

Electrical phenomena at interface:

The electrical double layer, electrokinetic phenomena, quantitative treatment of electro osmosis, Electrophoresis and streaming potential.

Unit 5 (15L)

Electrode processes:

Dissolution and deposition potential, decomposition potential and its determination, Concentration Polarization and over voltage(hydrogen overvoltage and oxygen overvoltage), The Limiting current density, Dropping Mercury Electrode.

- 1. Thermodynamics for Chemists by S. Glasstone.
- 2. An Introduction of Chemical Thermodynamics by R.P.Rastogi and R.R. Mishra.
- 3. Thermodynamics by K.S. Pitzer
- 4. Electrochemistry by S. Glasstone
- 5. Electrochemistry by Potter
- 6. Modern Electrochemistry by Bockris Reddy Vol I&II
- 7. Comprehensive Physical Chemistry by N.B. Singh, S.S. Das and N.S. Gajbhiye, New Age International Publishers.

(4 Credits) (60L)

Unit-1 (15L)

Structures of 2 to 8 Coordinate Metal Complexes:

Cation-anion ratio in various polyhedral, Hybrid orbitals and preferred conditions of formation of the complexes of following geometries :

C.N.2 - Linear

C.N.3 - Trigonal planar, Trigonal pyramidal

C.N.4 - Tetrahedral, Square planar

C.N.5 - Trigonal bipyramidal, Square pyramidal, pentagonal.

C.N.6 - Octahedral, Trigonal prism

C.N.7 - Pentagonal bipyramidal, Capped octahedral, Capped trigonal prism.

C.N.8 - Cubic, Tetragonal antiprismatic, Dodecahedral, Hexagonal bipyramidal, and Bicapped trigonal prism,

Stereochemical non-rigidity in four to eight coordinate Complexes.

Unit-2 (10L)

Stereoisomerism in six coordinate octahedral complexes (Ma3bcd, Ma2bcde, Mabcdef and complexes containing bi-and ter- dentate ligands, Intermolecular and intramolecular rearrangements (Bailar and Ray Dutta twist only), mechanism of racemisation in tris (chelate) octahedral complexes, Methods of resolution of optical isomers.

Unit-3 (10L)

Kinetics and mechanism of substitution reactions in octahedral Co (III) and square planar Pt (II) complexes.

Unit-4 (10L)

Mechanism of one electron transfer reactions (inner and outer sphere mechanisms), Factors affecting the rates of direct electron transfer reactions and the Marcus equation, Two electron transfer reactions.

Unit-5 (15L)

Metal Ligand Equilibria in Solution:

Step wise and overall formation constants and their relations, Factors affecting the stability of metal complexes with reference to the nature of metal ions and ligands, determination of stability constants by pH-metric and spectroscopic methods.

Books Recommended:

- 1. Inorganic Chemistry, 4th Edition, Principles of Structure and Relativity by J.E. Huheey, E.A. Keiter and R.L. Keiter, 1993
- 2. Chemistry of Elements by N.N. Greenwood and A. Ernshaw, Butterworths, 1997
- 3. Mechanism of Inorganic Reactions; A Study Of Metal Complexes in Solution by F. Bosolo and R.G. Pearson
- 4. Ligand Field Theory And Its Application by B.N. Figgis and M.A. Hitchman, Wiley, New York, 2000.

CH-204: Natural Products

	(4 Credits) (60L)
Unit-	- 1	(10L)
	ogenins: Classification, general method of structure determination of,	(-)
a.	Flavones- Chrysin	
b.	Flavonols – quercetin	
C.	Anthocyanins- Cyanin	
d.	Anthocyanidins- cyanidin chlorides	
Unit-	-2	(15L)
Terp	enoids: Introduction, isolation and general methods of determining structure of,	
a.	Monoterpenoids	
i.	Acyclic monoterpenoids: Citral and geraniol	
ii.	Monocyclic monoterpenoids : α -Terpineol	
b.	Diterpenoids	
	Abietic acid	
Unit-	-3	(15L)
Alka	loids : Introduction and general methods of determining structure of,	
i.	Hemlock alkaloid- Coniine	
ii.	Pyrrolidine-Pyridine alkaloid- Nicotine	
iii.	Chincona alkaloids -Quinine	
iv.	Opium alkaloids : Papaverine and Morphine	
v.	Rauwolfia alkaloids : Reserpine	
Unit-	-4	(08L)
	ohydrates: Structure and functions of,	(002)
	Disaccarides- Lactose, Sucrose	
ii.	Polysaccarides- Cellulose, starch	
Unit-	- 5	(12L)
	ynthesis of natural products:	()
i.	The acetate hypothesis, Isoprene rule, mevalonic acid from acetylco-enzyme – A,	
	biogenesis of terpenoids	
ii.	Shikimic acid pathway of biogenesis of aromatic ring	
iii.	General biogenesis of alkaloids	
Refe	rence Books:	
1.	Organic Chemistry, I.L. Finar Vol. I and II, 2000	
2.	Natural Products, S.M. Chawla, 2018	
3.	Biochemistry-Lehninger, 2000	

4. Biochemistry by L. Stryer, 1995

CH-205: Practical and Seminar

(8+ 1 Credits) (24h/week)

Marks (Practical): 200; Time: 12h in two days; Marks (Seminar): 25

Marks distribution (Practical)

Physical: 40

Inorganic: 40

Organic: 40

Viva: 30

Record: 20

Internal Assessment: 30

Physical Chemistry exercises:

- 1. Solubility curve for water-acetic acid-chloroform systems
- 2. Determination of the rate constant of the acid-catalysed hydrolysis of ethyl acetate at laboratory temperature
- 3. Determination of the rate constant of the hydrolysis of ethyl acetate by sodium hydroxide at laboratory temperature
- 4. Conductometric titration between strong acid and strong alkali
- 5. Determination of the dimerization constant of benzoic acid in benzene medium by partition method
- 6. pH measurement and pH titration of strong acid and strong base Study the adsorption of oxalic acid on charcoal and draw the Freundlich isotherm

Inorganic:

Either both gravimetric and one volumetric, one gravimetric estimation of two metal ions from following mixtures:

- a. Cu⁺² and Ni⁺²
- b. Cu^{+2} and Zn^{+2}
- c. Ni⁺² and Zn⁺²
- d. Cu⁺² and Ba⁺²
- e. Cu⁺² and Ag⁺
- f. Fe⁺² and Ag⁺
- g. Ba+2 and Ag+

Organic:

- 1. Analysis of primary binary organic mixture (Liquid-Liquid, Liquid-Solid, Solid-Solid)
- 2. Determination of equivalent weight of organic acids by direct titration method

Semester-III

CH-301: Spectroscopy-I

(4 Credits) (60L)

(15L)

Unit-1

UV-Visible Spectroscopy

Different type of electronic transitions, Lambert-Beer's law, Chromophores, Auxochromes, Solvent effect, Red shift and blue shift, Woodward's rule for conjugated cyclic and acyclic dienes and α , β – unsaturated Absorption in aromatic compounds (substituted benzene, naphthalene and carbonyl compounds, anthracene), Problems related to UV-Visible Spectroscopy.

Unit-2 (15L)

Infrared Spectroscopy:

Linear harmonic oscillator, Vibrational energies of diatomic molecules, Zero point energy, Force constant and bond strength, Anharmonicity, Morse potential energy diagram, Vibration rotation spectroscopy, P, Q, R branches, Breakdown of Born-Oppenheimer approximation, Selection rules, Overtones, Hot bands, Absorption by common functional groups, Brief description of IR and FTI.R instruments, Problems related to IR Spectroscopy.

Unit-3 (10L)

Raman Spectroscopy:

Theories of Raman Effect, Conditions of Raman active vibrations, Selection rules, Polarized and depolarized Raman lines, Study of: (a) Simple molecules such as SO₂, CO₂, N₂O and C₂H₂; (b) Hydrogen bonding and (c) Metal ions in solution, Mutual exclusion principle, Problems related to Raman Spectra and its interpretation.

Unit-4 (15L)

Diffraction Methods for Structure Determination

- a. X-ray Diffraction: Principle, elucidation of crystal structure of NaCl by X-ray diffraction, Structure factor, Methods for structure determination by trial and error methods, Fourier's method of analysis and Patterson's function method.
- b. Electron diffraction: Principle, technique, scattering intensity versus scattering angle curves, Wierl equation, energy electron diffraction (LEED)
- c. Neutron diffraction: Principle, technique and difference with electron diffraction

Unit-5:

Common problems related to above spectroscopic techniques

(05L)

- Fundamentals of Molecular Spectroscopy, 4th Ed. Mc Graw-Hill, C.N. Banwell 1.
- 2. Basic Principles of spectroscopy, Mc Graw -Hill, R. Chang
- Organic Spectroscopy, ELBS, W. Kemp
- Modern Spectroscopy, Wiley, J.M. Hollas

(4 Credits) (60L)

Unit-1 (15L)

Symmetry Properties and Quantum Mechanics

Invariability of schrodinger Equationfor a molecule with respect to symmetry operations and its consequences. Construction of molecular orbitals of ammonia and pie molecular orbitals of naphthalene, The direct product representation and its application in the derivation of selection rules for electronic, vibrational and Raman spectra

Unit-2 (15L)

Huckel Molecular Orbital Theory Of con jugated systems and its Applications

Calculation of energy levels and delocalisation energy of butadiene, cyclic conjugated systems: cyclopropenyl, cyclobutadiene, cyclopentadienyl, benzene, brief idea about delocalization energies of tropylium radical and cyclooctatetraene, concept of aromaticity and antiaromaticity, Huckel treatment of linear polyenes.

Unit-3 (15L)

Semi- Empirical and Ab-Intio SCF Theories

Hartee-Fock Self consistent (SCF) method, S emi- empirical SCF theory (CDNO, INDO & MNDO), Slater and Gaussian type orbitals, Configurational interaction and electron correlation, Moeller- Plasset Perturbation methods.

Unit-4 (10L)

Introduction to Density Functional Theory:

Concept of basis sets, exchange- correlation energy, The Hohenberg variational theorem and Kohn- Sham orbitals, The Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA). Density Functional theory and it significance.

Unit-5 (05L)

Molecular Mechanics

A brief introduction to molecular mechanics.

- 1. Introductory Quantum Chemistry by A. K. Chandra
- 2. Quantum Chemistry by R. K. Prasad
- 3. Molecular Quantum Mechanics by Atkins and Friedman
- 4. Quantum Chemistry by Ira N. Levine, Prentice Hall of India, New Delhi 1995
- 5. Chemical Application of Group Theory by F. A. Cotton

CHI-302: Chemical Application of Symmetry and Group Theory

(4 Credits) (60L)

Unit-1 (10L)

Symmetry and Point Groups

Definitions, the symmetry point groups, identification of molar point groups, molecules of low symmetry, high symmetry and special symmetry (C_n , S_n , D_n , C_{nv} , and D_{nh} only)

Groups, Sub-Groups, Classes and Matrices Representation

Definitions, multiplication tables, group generating elements, sub-groups and classes, irreducible representations, the orthogonality Theorem.

Matrix Representations of symmetry elements, block-factorization of larger matrices, matrix representation of C_{3v} , and C_{4v} , point groups, transformation matrices.

Normal Modes of Vibrations

Cartesian Coordinate and internal coordinate methods of normal mode analysis applied to C_{2v} (Symmetric XY₂, ZXY₂), C_{3v} (XY₃), T_d (XY₄) and O_h (XY₆) systems.

Valence Bond treatment and Molecular Orbitals

Formation of hybrid orbitals of XY_3 (planar), XY_4 (tetrahedral and square planar), Molecular Orbitals of A_2 and AB_n (n= 1 to 3) type molecules.

Crystal Fields

Derivation of 'd' orbital splitting patterns of central atom (M) in ML_2 , ML_3 , ML_5 , and ML_7 system (energy calculations are not required). The effect of weak crystal field on S, P, D, F and G spectroscopic terms in Oh and Td point groups.

Books Recommended:

- 1. F. A. Cotton, "Chemical aAplications of Group Theory". 2nd Ed..Wiley Eastern. 1971.
- 2. L. H. Hall, "Group Theory and Symmetry in Chemistry", McGraw Hill Inc.. 1969.
- 3. M. Orchin and H. H. Jaffe, "Symmetry, Orbitals and Spectra, Wiley Interscience. 1971.
- 4. C.J. Ballhausen and H. B. Gray, "Molecular Orbital Theory", W. A. Benzamin Inc. 1965.
- 5. K.Veera Reddy," Symmetry and Spectroscopy of Molecules", New Age International Limited Publisher, New Delhi.

CHO-302: Stereochemistry

(4 Credits) (60L)

Unit-1 (15L)

Stereoisomerism with chiral centre:

Element of symmetry, chirality, molecules with more than one chiral centers, threo and erythro isomers, interconversion of Fischer, Newman and saw-horse projections and configurational projections R/S and E/Z.

Unit-2 (15L)

Stereoisomerism with axial/planar chirality and Helicity:

Principle of axial and planar chirality; optical isomerism of biphenyl, allenes and spiranes; optical activity due to intramolecular crowding and absolute configuration.

Unit-3

a. Topocity and pro-stereoisomerism:

(05L)

Introduction; homotropic, enantiotropic and diastereotropic atoms, groups and faces; Nomenclature and symbols.

b. Cyclostereoisomerism

(10L)

Configuration and conformations; stability of mono- and disubstituted cycloheaxanes and cyclohexanones, Chirality of disubstituted cyclohexane, decalines and decanols.

Unit-4 (10L)

Assymetric Synthesis:

- **a.** Regioselective, stereoselective and sterospecefic reactions.
- **b.** Asymmetric synthesis involving chiral auxillary, chiral reagent and chiral catalysis.
- **c.** Enantioimeric excess, quasirecemateoptical purity.

Unit-5 (05L)

Stereochemistry of compounds containing S and P atoms and geometrical isomerism of compound containing C=N and N=N-bonds.

- 1. Stereochemistry of carbon compounds by E. L. Eliel, 1997
- 2. Stereochemistry by P. S. Kalsi, 1997
- 3. Stereochemistry of Organic compounds By D. Nasipuri, 1994

CHP-303: Electrodics and Electrocchemical Phenomena

(4 Credits) (60L)

Unit -1 (15L)

Conductance in non-aqueous media

Ion dissociation, its effect on conductance, diffusion of electrolytes, measurements of diffusion coefficient, in relation to conductance

Electrical Double Layer Theory

The Helmholtz –Perin Theory, The Gouy- Chapman Theory, Stern Modification in the Gouy-Chapman Theory.

Electrodics

The equilibrium exchange current density, Butler Volmer Equation, Tafel plot, high field and low field approximation, Electrodeposition and electropolymerization.

Corrosion

The mechanism of corrosion of metals, corrosion current and corrosion potential, Electrochemical corrosion theory, estimation of corrosion rates, corrosion prevention.

Polarization Resistance

Polarisation, Classification of polarisation phenomena, polarisation curves, Polarisation resistance and linear polarisation.

- 1. Electrochemistry by S. Glasstone
- 2. Electrolytic Solutions by Robinson& Stokes
- 3. Electrochemistry by Potter
- 4. Modern Electrochemistry by Bockris and Redd: Vol I and II
- 5. Electro Chemical Impedance Spectroscopy by Mc Donald
- 6. Theoretical Electrochemistry by L.I. Antropov

CHI-303: Coordination Chemistry

(4 Credits) (60L)

Unit-1 (13L)

Energy levels in an atom:

Relation between electronic configuration and energy terms, Hund's rules and ground state energy terms. Inter electron repulsion parameter. Variation of Racah B and C parameters in different transition series. Spin orbit coupling parameters.

Free ions in crystal fields:

Effect of weak crystal field on free ion terms in octahedral, square planar and tetrahedral symmetries. Orgel diagrams, Mixing of terms, Medium and strong field approximation in Oh point group, transition from weak to strong field and correlation diagram for only d² case, Noncrossing rule, Tanabe Sugano diagrams.

Electronic spectra of complexes:

Interpretation of the spectra of aqueous solution of $[M(H_2O)_6]^{n_+}$, calculation of Dq, B and β parameters, Jahn Teller distortion and its effect on electronic spectra.

Magnetic properties of Complexes:

Dia, para, ferro and antiferromagnetism, Quenching of orbital angular momentum by ligand . The magnetic properties of A, E and T terms.

Metal-ligand Bonding:

Limitations of CFT, Nephelauxetic series, molecular orbital energy level diagram of octahedral, tetrahedral and square planer complexes.

Books recommended:

- 1. B.N. Figgis, M.A. Hitchman, Ligand Field Theory and Its Applications, Willey, New York, 2000
- 2. D. Sutton, Electronics Spectra of Transition Metal Complexes, Mc-Graw-Hill, London, 1968.
- 3. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, New Age Inter Pvt. Ltd., New Delhi, 1999.

CHO-303: Pericyclic and Rearrangement Reactions

(4 Credits) (60L)

Unit-I (10L)

Carbocation rearrangements:

Pinacol- pinacolone, Wagner- Meerwein, Tiffeneau- Demjanov & Dienone- phenol rearrangements.

Unit-2 (10L)

Carbanion rearrangements:

Sommelet- Hauser, Stevens, Favorskii and Wittig rearrangements.

Unit-3 (10L)

Rearrangements to electron deficient N- and O-atoms

Hoffmann, Curtius, Lossen, Schmidt, Beckmann rearrangements & Baeyer-Villiger oxidation

Unit-4 (05L)

Miscellaneous rearrangements:

Wolff, Vinylcyclopropane-cyclopentene and benzidine rearrangements.

Unit- 5 (25L)

Characteristics and classification of pericyclic reactions. Conservation of M. O's symmetry, correlation, FMO and PMO methods forthe study of following reactions:

- **a. Electrocyclic reaction**: Study of linear conjugated dienes and trienes systems
- **b. Cyclo-addition reaction:** [2+2] and [4+2] systems, detailed study of Diel's-Alder reaction
- c. **Sigmatropic shift:** Study of [1,3]; [1,5] and [3,3] and higher order sigmatropic shifts Claisen –rearrangement; Cope, oxy-Cope and aza-Cope's rearrangements
- **d. Chelotropic and Group transfer reactions**. General introduction and mechanism.

- 1. Advanced Organic Chemistry Part. A & B By F. A. Carey and R. J. Sundberg, Plenum Publisher ,New York, 2007
- 2. Organic chemistry By J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxford University Press , New York, 2007
- 3. Advaced Organic Chemistry By J. March, 2007
- 4. Pericyclic Reactions By Mukharjee and Singh, 2001

CHP-304: Thermodynamics and Intermolecular Forces (4-Credits) (60L)

Unit-1 (07L)

Intermolecular Forces

Dispersion, dipole, induction and Charge transfer forces, The hydrogen bond.

Unit-2 (15L)

Thermodynamics of Mixture

Excess thermodynamic functions, Regular solutions, Solution of macromolecules, Activity Coefficient determination by NRTL (Non Random Two Liquids) and UNQUAC (Universal Quasi chemical Approach) Models, ASOG (Analytical Solvents of Groups) and UNIFAC (Universal functional Activity Coefficient) methods.

Unit-3 (15L)

Phase Equilibria

Thermodynamic relations at lamda - point. Thermodynamic interpretation of phase diagrams: Eutectic systems, Systems exhibiting complete miscibility in solid and liquid phases, Mixtures having a congruent melting point, Critical solution mixing.

Unit-4 (08L)

Liquid State

Configurational entropy and free energy, Cell theory of liquid state, Hole theory, Molecular theory of liquid viscosity, mesomorphism.

Unit-5 (15L)

Thermodynamics of Irreversible Processes

Entropy production in irreversible processes, Entropy equation for heat flow, relation between fluxes and forces, non- equilibrium stationary states, Linear phenomenological equations, Onsager's reciprocity relation, non –linear thermodynamic treatment of electro- kinetic phenomena, thermo- osmosis and reverse osmosis.

- 1. Introduction to thermodynamics of irreversible processes by I. Prigogine.
- 2. Non Equilibrium Thermodynamics in Biophysics by A. Katchalsky and P.F. Curran.
- 3. Thermodynamics of Irreversible processes by S.R. DeGroot.
- 4. Thermodynamics by E.A. Guggenheim.
- 5. Introduction to Non Equilibrium physical chemistry by R.P. Rastogi.
- 6. Thermodynamics-A core course by R.C. Srivastava, Subit K. Saha and A.K. Jain.
- 7. The Thermodynamics of Steady States by K.G. Denbigh.
- 8. Thermodynamics by Pitzer.
- 9. Regular solutions by J.H. Hilderbrand and R.L. Scott.

CHI-303: Supramolecular Chemistry

(4 Credits) (60L)

Unit-1 (20L)

Definition, classification of supramolecular host-guest compounds, nature of supramolecular interactions, Chelate and macrocyclic effects, General principles of molecular recognition, complex formation and host design, templates and self assembly.

Unit-2 (10L)

Host-Guest Chemistry (Cation Binding Hosts):

- i. Crown ethers
- ii. Cryptands
- iii. Spherands

Unit-3 (8L)

Host-Guest Chemistry (Anion Binding Hosts):

- i. Expanded porphyrins
- ii. Guanidinium Based reseptors

Unit-4 (8L)

Host-Guest Chemistry (Neutral Molecules Binding Hosts):

- i. Solid State Clatharates
- ii. Zeolites

Unit-5 (14L)

Selected Applications in:

- a. Catalysis
- **b.** Ion Transport
- **c.** Molecular switches, rectifiers and Molecular wires

Books Recommended

- 1. Supramolecular Chemistry: concepts and perspectives by J. M. Lehn, 1995
- 2. Supramolecular Chemistry by JW Steel and JL Atwood, 2004
- 3. Principles and Methods in Supramolecular Chemistry by H Scheneider and A Yatsimirsky, 2000
- 4. Supramolecular Chemistry: an Introduction by F Vogtle, 1993
- 5. Perspectives in Supramolecular Chemistry, Vol.2, Crystal Engineering and molecular recognition by Desiraju (Ed.), 2003

CHO-304: Biomolecules

(4 Credits) (60 L)

Unit-1 (15 L)

Water Soluble Vitamins:

Structure and Physiological functions of the followings water soluble vitamins-

- a. Non B- Complex Vitamin Vitamin C
- b. **B-Complex Vitamins** Thiamine B₁, Riboflavin B₂

Unit- 2 (10L)

Fat Soluble Vitamins:

Structure and Physiological functions of the followings fat soluble vitamins.

a. Vitamin A: Retinolb. Vitamin E: Tocoferol

c. Vitamin K: Vitamin K₁

Unit-3 (10 L)

Steroidal Hormones:

- a. General introduction to estrogens and androgens
- b. Oestrone (Estrone): Structure and synthesis, relationship to Oestradiol (estradiol)
- c. Progesterone: Preparation from steroid and physiological functions

Unit- 4 (10 L)

Non Steroidal Hormones

Structure and Physiological functions of Thyroxin and Adrenalin

Unit- 5 (15 L)

Steroids:

Diels hydrocarbon, Determination of ring system, positions of hydroxyl group, angular methyl group, double bond, nature and position of side chain in cholesterol, synthesis of cholesterol

- 1. Biochemistry by Lehninger, 2007
- 2. Organic Chemistry by I. L. Finar Vol. II, 2004
- 3. Biochemistry by Lubert Stryer, 2008

CHP-305: Practical and Seminar

(8+1 Credits) (24h/week)

Marks (Practical):200; Time: 12h in two days; Marks (Seminar): 25

Marks distribution (Practical)

Practical: 120 marks (Two practical of 60 marks each)

Viva: 25 Record: 25

Internal Assessment: 30

Excercises:

1. pH-metry:

- a. Determination of strength of strong acid and strong base
- b. Determination of strength of weak acid by pH-titration with a strong base
- c. Verification of Henderson's equation

2. Conductometry

- a. Equivalent conductance of strong electrolytes at infinite dilution
- b. Conductometric titration of weak acid with strong base
- c. Titration of mixtures of acids
- d. Precipitation titration
- e. Verification of Ostwald's dilution law
- f. Verification of Kohlrausch's law

3. Potentiometry

4. CMC of Surfactants by surface tension measurement

CHI-305: Practical and Seminar

(8+1 Credits) (24h/ week)

Marks (Practical): 200; Time: 12h in two days; Marks (Seminar): 25

Marks distribution (Practical)

Practical: 120 marks (Two practical of 60 marks each)

Viva: 25

Record: 25

Internal Assessment: 30

Exercises:

1. Gravimetric estimation of three metal ions from following:

2. EDTA Titration:

Estimation of Mg^{+2} , Zn^{+2} , and Mg^{+2} , Ca^{+2} in admixture.

CHO-305: Practical and Seminar

(8+1 Credits) (24h/ week)

Marks (Practical): 200; Time: 12h in two days; Marks (Seminar): 25

Marks distribution (Practical)

Practical: 120 marks (Two practical of 60 marks each)

Viva: 25

Record: 25

Internal Assessment: 30

Exercises:

1. Multistep synthesis of organic compounds

2. Estimation of sulphur in organic compounds

3. Estimation of glycine

Semester-IV

CH-401: Spectroscopy-II

(4 Credits) (60L)

Unit-1 (12L)

Mass Spectrometry

Measurement technique (El, Cl, FD and FAB), Molecular base and molecular ions, various class of organic molecules, McLafferty re-arrangement and retro-Diels-Alder Fragmentation, nitrogen rule and determination of molecular composition of organic compounds from mass spectra data.

Unit-2 (20L)

¹H-NMR

The spinning nuclei, Chemical shift and its measurement, factors affecting chemical shifts, anisotropic effect and shielding mechanism, interpretation of protons spin-spin coupling, coupling constant, simple, virtual and complex coupling, Chemical and magnetic equivalence, first and non-first order spectra, Analysis of AB, AMX and ABX systems, Simplification of complex spectra and NOE deuterium exchange, hindered rotation and rate process, NMR studies of other nuclei e.g., ¹⁹F and ³¹P, application in structural determination of simple organic and inorganic molecules.

Unit-3 (10L)

¹³C-NMR

General introduction, peak assignments, chemical shift, ¹³C-¹H coupling, Off-resonance Decoupling, Deuterium, fluorine and phosphorus coupling, NOE and DEPT, 2D NMR, Application to simple organic and inorganic molecules.

Unit-4 (10L)

Electron Spin Resonance Spectroscopy

Basic principle, factor affecting value, isotropic and anisotropic hyperfine coupling constant, Application to organic free radical, Methyl free radical, Naphthalene and Benzene free radicals, CID NP.

Unit-5 (8L)

Mossobauer Spectroscopy

Theory, Instrumentation, Applications - isomer shift, nuclear quadrupole coupling and hyperfine interaction, Problems related to Mossobauer Spectroscopy.

- 1. Fundamentals of Molecular Spectroscopy, 4th Ed. Mc Graw-Hill, C.N. Banwell
- 2. Basic Principles of spectroscopy, Mc Graw -Hill, R. Chang
- 3. Organic Spectroscopy, ELBS, W. Kemp
- 4. Modern Spectroscopy, Wiley, J.M. Hollas

CHP-402: Chemical Kinetics, Solid state and Reaction Dynamics

(4-Credits)(60L)

Unit-1 (15L)

Chemical Kinetics

The study of fast reaction: Flow system, Relaxation and shock tube methods, Flash photolysis

Unit-2 (15L)

Oscillatory Chemical Reactions

Autocatalysis, Autocatalytic Mechanisms of oscillatory chemical reaction: The lotka Volterra mechanism, The Brusselator, the Oregonator, Bistability and Chemical chaos.

Unit-3 (10L)

Solid State

Thermodynamics of Schottky and Frankel Defects, Synthesis, Characterization and Applications of Nanomaterials; Solid State Reaction.

Unit-4 (15L)

Statistical Treatment of Unimolecular reaction

Limitation of Lindemann theory, Hinshelwood treatment, RRK theory (salient features and limitations) RRKM theory and advances made by Slater.

Unit-5 (05L)

Reaction Dynamics

Collision cross-section, Inter- molecular potential, potential energy surfaces and elastic molecular collisions.

- 1. Solid State Chemistry by D.K. Chakrabarty. New Age International (P) Limited, Publishers, New Delhi.
- 2. Molecular Reaction Dynamics by R.D. Levine, R.B. Bernstein.
- 3. Dynamics by N. Sathyamurthy
- 4. Theories of Chemical Reaction rate by K.J.Laidler.
- 5. Physical Chemistry, Walter J. Moore

CHI-402: Bioinorganic Chemistry

(4 Credits) (60L)

Unit-1 (15L)

Metalloenzymes:

Zinc enzymes - carboxypeptidase, carbonic anhydrase; Copper enzymes - superoxide dismutase; Mobybdenum - xanthine oxidase; Coenzyme vitamin B_{12} , Biological nitrogen fixation, molybdenum nitrogenase, other nitrogenase model systems.

Bioenergetics and ATP cycle:

Glucose storage, metal complexes in transmission of energy, chlorophylls, Photosystem I and II in cleavage of water.

Transport and Storage of Dioxygen:

Heme proteins and oxygen uptake, Structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, model synthetic complexes of iron.

Electron Transfer, Metal Storage and Transport:

Structure and function of metalloproteins in electron transport process - cytochromes and iron - sulphur proteins, synthetic models, Ferritin, transferrin and siderophores. .

Metals in Medicine:

Metal deficiency and diseases, toxic effects of metals, metals in chemotherapy with particular reference to anticancer drugs.

Books Recommended:

- 1. Bioinorganic Chemistry. R. N. Hay. Wiley. 1984.
- 2. The Inorganic Chemistry of Biological Processes. M. M. Hughes. Wiley 1981.
- 3. An Introduction to bioinorganic Chemistry. El Ichiro Ochai. Allyn. 1977.
- 4. Inorganic Chemistry: Principles of structure and reactivity. J.E. Huheey Harper. 1983.
- 5. Advanced inorganic Chemistry. F.A. Cotton and G. Wilkinson. Wiley. 1999.

CHO-402: Organic Synthesis

(4 Credits) (60 L)

Unit-1 (18 L)

Selective named reactions and their applications in organic synthesis:

Barton, Bayllis–Hillman, Ene, Hoffmann-Lofferer-Fretag, Michael addition, Mitsonubu, Nazaro Mannich, Julia & Peterson olefination, Robinson annulations, Reformatsky, Shapiro, Storkenamine and Woodward-Prevost hydroxylation

Unit-2 (10L)

Oxidation:

Scopes of the following reagents with applications and mechanisms: SeO_2 , Jones reagent, PCC, PDC, Swern oxidation and iodobenzene diacetate.

Unit-3 (10 L)

Reduction:

Scope,Mechanism and stereochemistry of reduction with following reagents-NaBH₄, LAH, DIBALH, diborane, dis-isoamyl borane, 9-BBN and Birch reduction.

Unit- 4 (12L)

Reagents:

Preparation and uses of following reagents in organic synthesis.

- **a.** Gillman, DCC, DDQ, LDA, Diazomethane, Bu₃SnH /AIBBN,, Wilkinson catalyst. and 1,3-dithiane (unpolung)
- **b.** Sulphur and phosphorous Ylids.

Unit -5 (10L)

Pd(0) and Pd(II) complex in organic synthesis: Heck, Suzuki, Stille and Sonogashira reactions,

- 1. Organic Synthesis By Michael B Smith, Mc-Graw Hill, 2001
- 2. Advanced Organic Chemistry Part. A & B By F. A. Carey and R. J. Sundberg, Plenum Publisher, New York, 2002
- 3. Advanced Organic Chemistry By J. March, 2007
- 4. Organic chemistry By J. Clayden, N. Greeves, S. Warren and P Wothers, Oxford University Press, New York, 2007

CHP-403: Statistical Mechanics

(4-Credits)(60L)

Unit-1 (15L)

Basic of Classical Statistical Mechanics

Phase space, Ensembles-average, Liouvilles theorem, Basic postulates, Classical limit, Quantisation of phase space.

Unit-2 (10L)

Distribution laws

Energy levels, Boltzmann distribution law, Fermi-Dirac statistics Bose –Einstein Statistics.

Unit-3 (10L)

Distribution & Thermodynamics

The partition functions, relation of the partition function of the thermodynamic function.

Unit-4 (15L)

Determination of Partition functions

Localised and non-localised systems, Separation of the partition function. Translation partition function. The Sackur Tetrode-equation, Rotational partition function, vibrational partitionfunctions, Electronic partition function. Derivation of thermodynamic properties of ideal gases from partition functions.

Unit-5 (10L)

Applications

Equilibrium Constants from partition function for: Isomerisation equilibrium, Ionisation equilibrium ($H \leftrightarrow H^++e$), and Dissociation equilibrium($Na_2 \leftrightarrow 2Na$)

- 1. Statistical Mechanics: N. Davidson
- 2. Statistical Mechanics: D.A. Mcquarrie
- 3. Thermodynamics: J.P. Holman
- 4. Theoretical Chemistry: S. Glasstone
- 5. Physical Chemistry: Fried, Blukis and Hameika

CHI-403: Organotransition Metal Chemistry

(4 Credits) (60L)

Unit-1 (07L)

Alkyls and Aryls of Transition Metals:

Types, General Synthetic Routes, Stability and Decomposition pathways.

Unit-2 (08L)

Compounds of Transition Metal - Carbon Multiple Bond: Carbenes and Carbynes:

Low valent carbenes and carbynes ,synthesis, nature of bond and Structural Characteristics.

Unit-3 (25L)

Transition Metal π - Complexes:

- a. Preparations, Important reactions relating on the ligands, Structural features and bonding of alkenes, alkynes, allyls, diene, dienyl, arene complexes, MO approach of bonding in ferrocene and bis (benzene) chromium.
- b. Ligand behaviour of C₃Ph₃+, C₇H₇+ and C₈H₈²- in different organometallic compounds.
- c. Substitution reactions in metal carbonylsd using σ -donor, σ -donor and π -acceptor and π -donor ligands.

Catalysis involving organometallic compounds:

Olefin hydrogenation. Oxo reaction. Fischer Tropsch process. Wacker process. Polymerisation of olefins.

Fluxional Organometallic Compounds:

Fluxionality and dynamic equilibria in compounds such as η^3 – allyl and η^1 dienyl complex.

Books Recommended:

- 1. Comprehensive Organometallic Chemistry, Ed. E.W. Abel, Abel, F.G.A. Stone and G. Wilkinson, Pergamon, 1982.
- 2. Advnaced Inorganic Chemistry, F.A. Cotton and G. Wilkinson, 'Wiley, 1999.
- 3. The chemistry of elements, N.N. Greenwood and A. Earnshaw, 1997.
- 4. Inorganic Chemistry, principles of structure and reactivity. J.E. Huheey, Harper, 1983.
- 5. Organometallic Chemistry (A unified approach), R.C. Mehrotra and A. Singh, Wiley Eastern, 1991

CHO-403: Select Topics in Organic Chemistry

(4 Credits) (60 L)

Unit-1 (15L)

Aromaticity:

Concept of aromaticity, anti-aromaticity, non-aromaticity and homoaromaticity. Alternant and non-alternant systems. Aromaticity in non-benenoids (tropolone, azulene, annulenes, ferrocene and fullerene)

Unit- 2 (10L)

Protection and Deprotection of Groups:

Principle of protection and deprotection of alcohols, thiols and 1,3-diols, amines, carbonyls and carboxyl groups in organic synthesis.

Unit- 3 (08L)

Heterocycles:

General introduction and nomenclature. Chemistry of:

- **a. Five membered:** Pyrazole& imidazole; and thiazole&iso-thiazole
- **b. Six membered:** Pyrazine, pyrimidine and pyridaze

Unit- 4 (20L)

Organic Photochemistry:

Electronically exited states, spin-multiplicity, Jablonski diagram

- **a. Photochemistry of Alkenes:** Geometrical isomerization, cyclic diamerization and photo-oxidation reaction. Reactions of 1,4 and 1,5- dienes (di-pi methane and related rearrangements)
- **b. Photochemistry of Aromatic compounds:** Isomerization, skeletal isomerization, isomerization of disubstituted benzenes. photo-Fries rearrangement.

Unit-5 (07L)

Photochemistry of Carbonyl compounds:

Reduction, inter and intramolecular addition (Patterno-Buchi) Fragmentation (Norish-1 and Norish-11).Reaction of saturated acyclic, cyclic and unsaturated carbonyl compounds.Photochemistry of cyclohexenone and cyclohexadienones

- 1. Advanced Organic Chemistry Part. A & B By F. A. Carey and R. J. Sundberg, Plenum Publisher, New York, 2007
- 2. Advanced Organic Chemistry By J. March, 2007
- 3. Organic chemistry By Clayden, Greeves, Warren and Wothers, Oxford University Press , New York, 2007
- 4. Molecular Reactions and photochemistry By C. H. Depay and O.L. Chapman, 2001

CHE- 404: Polymer Chemistry

(4-Credits) (60L)

Unit-1 (15L)

Basic Concepts and Polymer Characterization

General definition, Types and Classification of polymers, Concept of average molecular weights in polymers: (Number average, Weight average, Viscosity average and Sedimentation average molecular weights), Concepts of Mono-dispersity, poly-dispersity, Significance of Molecular Weight, Distribution Curves of polymers.

Unit -2 (15L)

Polymerization

Kinetics and mechanism of condensation, Addition (Radical chain and Ionic chain), Coordination and Copolymerization.

Unit-3 (10L)

Degradation of Polymers

Types of degradation: Random degradation and Chain depolymerisation, A general idea of thermal, mechanical and oxidative degradation, Antioxidants and stabilizers.

Unit -4 (10L)

Rheology of Polymers

Viscous flow (Newtonian and Non- Newtonian fluids), Rubber elasticity (thermodynamic and entropy, elasticity), Visco-elasticity, The glassy state and glass transition temperature.

Unit -5 (10L)

Polymer Processing

Plastic Technology: A general idea of Moulding and Extrusion techniques, Thermoforming and Thermofoaming.

Fiber Technology: A brief idea of textile and fabric terms and properties of fibers, Fiber Spinning techniques (melt, wet and dry spinnings).

- 1. F.W. Billmeyer, "Textbook of Polymer Science", John Wiley &Sons, New York.
- 2. H.R.Allcock, F.W.Lampe and J.E Mark, "Contemporary Polymer Chemistry", PearsonEducation Prentice Hall, Singapore.
- 3. Charles E. Cariaher, "Polymer Chemistry: An Introduction", Marcel Dekker Inc, New York.
- 4. U.R.Gowariker, N.V.Vishwanathan and J. Shreedhar, "Polymer Science", New Age International Publishers, New Delhi.
- 5. S.S.Das and N.B.Singh,An Introduction to Polymer Science and Technology", New age International Publishers, New Delhi.

CHE-405: Inorganic Materials

(4 Credits) (60L)

Unit-1 (10L)

Lattice Defects:

Introduction to types of solids, Perfect and imperfect crystals, point defects, line defect and plane defect (definition and explanation of meaning), Schottky and Frenkel defect, Nonstoichiometric defect (structural aspects), incorporation of stoichiometric excess defects, Magnetism due to defects (soft and hard magnetic materials).

Unit-2 (08L)

Synthesis of Inorganic Materials:

Synthesis of solid state materials using different techniques (ceramic techniques, co-precipiattion techniques, sol-gel techniques, precursor techniques).

Unit-3

Properties of Materials

a. Optical Properties

(10L)

Introduction, Optical properties of metals and non-metals, Luminescence, Photoconductivity, Lasers, non linear optical materials and optical fibers in communications.

b. Electrical Properties

(12L)

Electrical conduction, Conduction in term of free electron and band theory. Semiconductors -Intrinsic and Extrinsic semiconductors and semiconductor devices.

Introduction of superconductors, High Tc super conductivity in Cuparates, preparation and characterization of 1-2-3 and 2-1-4 materials, Theory of superconductivity. Application of high Tc materials.

Unit-4 (10L)

Nano Materials:

Introduction, preparation of nano materials, size property relationship, Carbon nanotubes, application of nano materials.

Unit-5 (10L)

Metal clusters:

Conditions for formation of metal-metal bond. Carbonyl type clusters. Electron count in metal clustures, Isopoly and heteropoly acids and salts of Cr, V, Mo.

Books Recommended

- 1. A.F. Wells, Structural Inorg. Chem., ELBS & Oxford Univ. Press, 1975
- 2. C.N.R. Rao, A Muller & A.K. Cheetham, The Chemistry of nano-Materials, Wiley-VCH, Vol. 1 and Vol. 2, 2004.
- 3. F.A. Cotton, G. Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorg. Chem., John-Wiley & Sons, 1999.
- 4. J.E. Huheey, G.A. Keiter, R.L. Keiter, Inorg. Chem.: Principles of Structures and Reactivity, Harper Collins College Publishers, 1993.
- 5. D.M. Bruce, Inorganic Materials, 5 Volume sets, Wiley, 2011.
- 6. U. Schbert, N. Husing, Synth. of Inorg. Materials, Wiley, 2005.
- 7. D. Bahadur, Inorg. Materials: Recent Advances, Alpha Science International Ltd., 2004.

CHE-406: Drugs and Agrochemicals

(4 Credits) (60 L)

Unit- 1 (15L)

Synthetic Drugs A:

A general methods of synthesis and applications of:

- i. Sulpha drugs: Sulphanilamide, sulphathiazole, sulphathalidine, sulphasuccidine, sulphaguanidine, sulphapyridine
- ii. Antimalarials: **(a)** 4-Aminoquinoline derivatives: chloroquine, santoquine **(b)** 8- aminoquinoline derivatives: Pamaquine, Pentaquine.

Unit- 2 (15L)

Synthetic Drugs B:

A general introduction and applications of:

- i. Anti-cancer agents: Nitrogen mustards, antimetabolites in cancer chemotherapy.
- ii. Psychopharmacological agents: Synthesis and applications of promazine, chloropromazine, mepazine.
- iii. Antitubercular agents: Synthesis and applications of Para Aminosalicylic Acid (PAS), Thiosemicarbazones, and hydrazides.

Unit-3 (10L)

Antibiotics:

Synthesis of penicillin-G, penicillin-V, chloramphenicol,

Unit-4 (06L)

a. Insecticides

- i. A brief reference to natural insecticides, tobacco alkaloid, pyrothrins and rotenoids (detailed chemistry not required)
- ii. Organophosphorus insecticides, OMPA, Parathion, malathion,
- iii. Halogenated insecticides , halogenated alkanes, gammexane, DDT and important analogs (DFDT, DMDT, DDD).

b. New breed of pesticides

(04L)

- i. JH analogues and anti JH compounds in pest control (detailed structure not required).
- ii. Use of sex pheromones in pest control

Unit- 5 (05L)

a. Fungicides:

Synthesis and applications of following agrochemicals Halogenated phenols and quinones, dithiocarbamates, Zineb, Maneb, Ferbam

b. Herbicides (05L)

Synthesis and applications of 2,4-D and related compounds, substituted ureas and carbamates

Reference Books:

Medicinal Chemistry by A. Burger, 2002

CHE-407: Solid State Chemistry

(4 Credits) (60L)

Unit-1 (07L)

Crystal Structures:

Rock salt, Zinc blende, Wurtzite, Daimond, Graphite, Fluorite, Sesquoide, Spinel (Normal/inverse), ReO₃, Perovskite, Amorphous state, quasi-crystals, Icosahedron, Silicates, Zeolites

Unit-2 (08L)

Imperfections in crystals:

Point defects: Schottky and Frenkel defects, Colour centres line defects: Edge and screw dislocations, Burger's vector, dislocation densities, dislocation multiplicity and slip dislocation and crystal growth.

Surface imperfection: Grain boundaries

Unit-3 (15L)

a. Semiconductors:

Intrinsic and impurity semiconductors, Carrier concentrations, Effect of temperature aon electrical conductivity and mobility of electrons in semiconductors, Hall effect, Seebeck coefficient, p-n junctions, Organic semiconductors

b. Superconductivity

Zero resistance and transition temperature, superconductivity and periodic table, Magnetic properties, Theory of superconductivity (BCS theory), Type I and Type II superconductors, Hard superconductors, Preparation of superconducting materials and their applications.

Unit-4 (15L)

Phase transformations in solids:

Classification and thermodynamics of phase transformations in solids, Experimental methods of the study of phase transformations, Phase transformations in metals, Nucleation and crystal growth mechanism, Alloys, Some compounds such as titanium dioxide, aluminium oxide, dicalcium and tricalcium silicate, Dendritic growth, Preparation of single crystals from vapour, melt and solution.

Unit-5 (15L)

Solid State Reactions:

Classification, Nature of solid state reactions, Reactions involving single solid phase, solid-gas reaction, solid-solid reaction, solid-liquid reaction, Intercalation chemistry, Reactions of organic solids, factors affecting solid state reactivity, Experimental methods for the study of solid state reactions

Reference Books:

- 1. Solid state chemistry and applications by A.R. West (2014. 2E)
- 2. Phase transitions in solids by K.J. Rao and C.N.R. Rao (1978)
- 3. Solid state chemistry by N.B. Hannay (1967)
- 4. Solid state chemistry by D.K. Chakrabarty (2010)

CHE-408: Nuclear and Radiation Chemistry

(4 Credits) (60L)

Unit-1 (07L)

The Atomic Nucleus:

The atom, Units used in Nuclear chemistry, The nucleus and the outer sphere, classification of nuclides, nuclear stability, atomic energy.

Unit-2 (08L)

Nuclear Models:

The shell model, The liquid drop model, The Fermi gas model, The collective model, The optical model.

Unit-3 (15L)

Nuclear Reactions:

Bethe's notation, types of nuclear reactions, conservation in nuclear reactions, reaction cross section, the compound nucleus theory, experimental evidence of Bohr's theory, Experiments of Ghoshal, Alexander and Simonoff, Specific nuclear reactions, Photonuclear reactions, Direct nuclear reactions, Thermonuclear reactions.

Unit-4 (15L)

Nuclear fission:

The process of nuclear fission, Fission fragments and their mass distribution, Charge distribution, Ionic charge of fission fragments, Fission energy, Fission cross-sections and thresholds, Fission neutrons, Theory of nuclear fission, The nuclear Reactors.

Unit-5 (15L)

Radioactivity:

Radioactive elements, General characteristics of radioactive decay, Alpha decay, Beta decay, Nuclear deexcitation, gamma emission, artificial readioactivity

The Szilard-Chalmer's reaction, Radiochemical principles in the use of tracers, Uses of nuclear radiations, Radioisotopes as a source of electricity

Reference Books

Essentials of Nuclear Chemistry by Hari Jeevan Arnikar (1995)

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CHE-409: Biophysical Chemistry

(4 Credits) (60 L)

Unit-1 (10L)

Biological Membranes:

Mechanism of facilitated diffusion of glucose, chloride ion and bicarbonate ion through erythrocytes, Mechanism of active transport of Na⁺, K⁺, Ca⁺² and proton through membrane, cotransport: symport and antiport, Brief description of Na⁺ channel protein and transport antibiotics. Brief description of molecular assembly and LB films

Unit-2 (20L)

a. Nucleic acids:

Conformation of DNA and RNA (A,B and Z forms), Genetic code and gene-protein relationship, DNA cloaning and principle of protein engineering, DNA damage and repair mechanism

b. Proteins:

Conformation of polypeptide chain, periodic structures in proteins: α -helix, β -pleated sheet, collagen helix and β -turn, principle of protein folding and forces involved in protein folding Structures and functions of myoglobin, haemoglobin, lysozyme and carboxypeptidase A.

Unit-3 (10L)

Bioenergetics:

The mechanism of oxidative phosphorylation-chemical coupling hypothesis, the conformational coupling hypothesis and chemi-osmotic coupling hypothesis

Unit-4 (10L)

Biological Regulations:

Prostaglandins, cyclic AMP and its role in hormone action, Interferon

Unit-5 (10L)

Enzyme Kinetics and Theory of Enzyme Catalysis:

Presteady state kinetics, steady state kinetics, kinetics of enzyme inhibitors and determination K_1 , kinetics of multisubstrate enzyme-compulsory order, random order and double displacement type mechanism, non-linear enzyme kinetics

Reference Books:

- 1. Biophysics by M.V. Vallenstein, MIR publication, Moscow
- 2. Biochemistry by L. Stryer, Freeman and Co,, San Fransisco (Indian Print CBS Publications, Delhi).
- 3. Biophysical Chemistry Part I, II and III by C.R. Cantor and P.R. Schimmel, Freeman and Co., San Fransisco.
- 4. Principles of Biochemistry by Lehninger, Neloson and COX, Worth Publishers INC, US (Indian Print CBS Publishers, Delhi)
- 5. Enzyme Kinteics by P.C. Engel, Chapman and Hall, London

CHE-410: Computational Chemistry

(4 Credits) (60L)

Unit-1 (05L)

Introduction to Computational Chemistry and computable quantities (structure, potential energy surface, chemical properties)

Unit-2 (10L)

Construction of z-matrix

- **a.** Diatomic molecules
- **b.** Polyatomic molecules
- c. Ring systems

Unit-3 (10L)

Force Field/Molecular Mechanics

Potential energy functional forms

- i. Common force fields viz., Harmonic, LJ (6-12), LJ(10-12) and More
- ii. Existing force fields in popular packages viz., AMBER, CHARMM, DREIDING and MMn

Unit-4 (15L)

Ab-initio HF calculations:

- a. Geometry optimization and calculation of HF energy
- **b.** Basis sets
- **c.** Density functional theory
- i. Basic theory
- ii. Advantage over Ab-initio approach
- iii. Gaussian, Gamess & MOLPRO
- iv. Applications

Unit-5 20L

Applications to Real systems

- **a.** Biomolecules
- i. Methods for modelling Biomolecules
- ii. Site-specific interaction
- iii. Introduction to computer aided Drug design (CADD)
- **b.** Synthetic route prediction
- **c.** Polymers/ smart materials
- **d.** Transition metals and clusters

Reference Books:

- 1. Introduction to computational chemistry by Frank, Jensen
- 2. Computational Chemistry by C.J. Cramer

CHP-411: Practical and Seminar

(8+1 Credits) (24h/week)

Marks (Practical):200; Time: 12h in two days; Marks(Seminar): 25

Marks distribution (Practical)

Practical: 120 marks (Two practical of 60 marks each)

Viva:25 Record: 25

Internal Assessment: 30

Excercises:

1. Chemical Kinetics

- a. Determination of rate constant of acid hydrolysis of esters
- b. Relative strength of strong acids by studying the kinetics of hydrolysis of esters
- c. Kinetics of reactions between potassium persulphate and potassium iodide
- d. Kinetics of iodination of acetone

2. Optical Methods

- a. Colorimetry: Verification of lambert- Beer's Law
- b. Refractometry
- c. Spectroscopic methods of analysis: UV-visible, IR
- d. Polarimetry

3. Electrodeposition of metals

CuSO₄, ZnSO₄

CHI-411: Practical and Seminar

(8+1 Credits) (24h/week)

Marks (Practical): 200; Time: 12h in two days; Marks (Seminar): 25

Marks distribution (Practical)

Practical: 120 marks (Two practical of 60 marks each)

Viva: 25 Record: 25

Internal Assessment: 30

Exercises:

A. Instrumentation:

1. Potentiometry

- a. Acid-Base, Redox Titrations.
- b. Determination of stability constants of suitable complex systems.

2. Conductometry

Acid-Base and precipitation Titrations

3. Colorimetry and Spectrophotometry:

Estimation of the following metals in solution V, Cr, Mo, Fe and Ni.

4. Flame Photometry:

- a. Estimation of sodium and potassium in admixture.
- b. Estimation of magnesium and calcium in tap water.
- c. Estimation of calcium in calcium salt solution.

B. Preparation and characterization of the following complexes:

- i. Tetramminecarbonatocobalt(III) chloride
- ii. Tetramminecarbonatocobalt(III) nitrate
- iii. Pentaminnechlorocobalt(III) chloride
- iv. Potassium trioxalatoferrate(III)
- v. Ammonium hexafluoroplumbate(IV)
- vi. Ammonium hexafluorostannate(IV)
- vii. Cobalt(II) tetrakis(thiocyanato)mercurate(II)
- viii. Tetramminedichlorocobalt(III) chloride
- ix. Tris(pyrazolinato)iron(III)

CHO-411: Practical and Seminar

(8+1 Credits) (24h/week)

Marks (Practical): 200; Time: 12h in two days; Marks (Seminar): 25

Marks distribution (Practical)

Practical: 120 marks (Two practical of 60 marks each)

Viva: 25 Record: 25

Internal Assessment: 30

Exercises:

1. Analysis of ternary organic mixture

2. Estimation of glucose

Deen Dayal Upadhyaya Gorakhpur University, Gorakhpur Academic Programmes under Ordinance Choice Based Credit System (CBCS)

1. Applicability

This ordinance shall apply to all P.G. programmes under the Choice Based Credit System (CBCS) and shall come into effect from the academic session 2019-20.

2. Definitions of Key Words:

- a) Academic Year: Two consecutive (one odd, July to December + one even, January to June) semesters shall constitute one academic year.
- b) Choice Based Credit System (CBCS): The CBCS provides choice for students to select from the prescribed courses (core and elective).
- c) Course: Usually referred to, as 'papers' is a component of a programme. All courses need not carry the same weightage. A course may be designed to comprise lectures/ tutorials/laboratory work/ field work/outreach activities/ project work/ vocational training/viva/ seminars/term papers/assignments/ presentations/ self-study etc. or a combination of some of these.
 - d) Credit Based Semester System (CBSS): Under the CBSS, the requirement for awarding a degree or diploma or certificate is prescribed in terms of number of credits to be completed by the students.
 - e) Credit: A unit by which the weightage of course work is measured. It determines the number of hours of instructions required per day. One credit is equivalent to one hour of teaching (lecture or tutorial) or two hours of practical work/field work per day.
 - f) Cumulative Grade Point Average (CGPA): It is a measure of overall academic cumulative performance of a student in all semesters.
 - g) Letter Grade: It is an index of the performance of students in a said course. Grades are denoted by letters O, A+, A, B+, B, C, P and F, Ab.
 - h) Grade Point: It is a numerical value allotted to each letter grade.
 - i) Programme: An academic programme leading to award of a Degree, diploma or certificate.

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- j) Semester Grade Point Average (SGPA): It is a measure of academic performance in a semester.
- k) Semester: Each semester will consist of academic work equivalent to 90 teaching days. The odd semester will be from July to December and even semester from January to June in every academic year.
- Transcript or Grade Card: The transcript/grade card will be given to all students upon completion of academic work of all semesters of a programme and will display the course details (code, title, number of credits) grade obtained in each course, and SGPA/CGPA.
- 3. (a) All P.G. programmes shall comprise of a minimum of four semesters.
 - (b) Each Semester shall comprise of a minimum of 5 (Five) courses/papers.
 - (c) In all, a student needs to complete a minimum of twenty courses of 5 credits each for being eligible to complete a P.G. programme.
 - (d) Thus, the minimal credit requirement for a P.G. programme am is 100 credits.

4. Types of Courses:

Courses in a programme may be of two kinds: Core and Elective.

- a) Core Course:-Such courses are to be studied compulsorily by a student.
- b) Elective Course:-Elective course is a course which may be chosen from a pool of elective courses offered by different departments. Elective courses may be Discipline-centric (intra-departmental) or/and Interdisciplinary (inter-departmental). They may be offered across all the four semesters.

5. Attendance requirement.

Students with less than 75% attendance in a course shall not be eligible to appear in the end Semester Examination. However, in exceptional cases the Head may grant a relaxation in required percentage of attendance by not more than 15 % on the basis of genuine reasons/ground.

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6. Programme Duration and Credit requirements:

SI. No.	Programme	Minimum number of	Course Duration
		credits	(In Years)
1	Post Graduate Degree	100	Two Years
	(Four Semester Course)		* ;

Note: The maximum duration of a programme will be four years.

7. Examination(s) and Assessment / Evaluation:

Evaluation will have two components, namely:

- i. Internal Assessment 30% weightage of a course.
- ii. End Semester Exam 70% weightage of a course. For the ease of evaluation while making a transition from marks based system to grading system, examination of each course of a semester will be held for maximum marks of 100 irrespective of number of credits allotted to the course (30 for internal assessment and 70 for end semester examination). There shall be no separate 'paper'/ course for the viva-voce. The viva-voce examination can, however, be component of the internal assessment.

The marks will be converted to grades as per the following table

Marks obtained	Grade	numeric value of grade
90 and above	0	10
80 and above but less than 90	A+	9
70 and above but less than 80	Α	8
60 and above but less than 70	B+	7
50 and above but less than 60	В	6
45 and above but less than 50	С	5
40 and above but less than 45	Р	4
less than 40	F	0
Absent	Ab	0

Rounding of the numeric value of grades obtained will be done till two places of decimal.

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Promotion and Degree Awarding Rules:

- A student obtaining F grade in any course shall be considered failed in that course.
- A student shall be allowed promotion to next year if both the following conditions are met by him/her:
 - i) His/Her CGPA is equal to or greater than 4.00.
 - ii) He/she does not have 'F' or 'Ab' grade in more than fifty percent courses of a Semester.
- Those students who are NOT eligible for promotion shall have to reappear in the end semester examination of all courses in the semester(s). However, the grades of internal assessment shall be carried forward in such cases.
- Those students who are eligible for promotion and wanting to improve their grades may avail opportunity to improve the grade within the maximum stipulated time period will be allowed to complete the programme. However, the grades of internal assessment shall be carried forward in such cases.

A student shall be deemed to have completed the degree requirements, if the student has:

- a. Passed all the prescribed Courses/Practicals/Field Work/Thesis/Projects/ Dissertations etc.
- b. Obtained the minimum required CGPA of 4.00 without 'F' or 'Ab' in any course.
- c. Those students who have achieved CGPA of 4.00 without 'F' and 'Ab' grade may avail opportunity to improve the grade within the maximum stipulated time period will be allowed to complete the programme. However, the grades of internal assessment shall be carried forward in such cases.
- d. Paid all the dues of the University and has no pending case of indiscipline.

Computation of SGPA and CGPA, and issue of Grade Card / Transcript

The Semester Grade Point Average (SGPA) and Cumulative Grade Point Average (CGPA) will be computed as follows:

a) Semester grade point average (SGPA)

The Semester grade point average (SGPA) is a weighted average of the grade points earned by a student in all the Courses credited and describes his/her Academic Performance in a Semester. If the grade points associated with the letter grades

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awarded to a student are g1, g2, g3gn in n courses and the corresponding weights (or credits of the courses) are w1, w2, w3.....wn the SGPA is given by: SGPA = (g1.w1 + g2.w2 + gn.wn) / (w1 + w2 ++ wn)

b) Cumulative Grade point average (CGPA)

The Cumulative grade point average (CGPA) indicates the overall academic performance of a student in all the courses registered up to and including the latest completed semester term. It shall be computed in the same manner as the SGPA, considering all the courses (say, n) and is given by: CGPA = (g1.w1 + g2.w2 ++ gn.wn) / (w1 + w2 +.....+ wn)

Whenever a student is permitted to repeat or substitute a Course, the new letter grade replaces the better of the old and new letter grades in the computation of the CGPA.

Awarding final grade from the CGPA. To be eligible for Degree minimum CGPA requirement is 4.00 with fulfilment of all requirements for the award of Degree.

Table-1

CGPA	Final grade	Meaning
10	0	Outstanding
9	A+	Excellent
8	A	Very Good
7	B+	Good
6	В	Above Average
5	С	Average
4	Р	Pass
0	F	Fail
0	Ab	Absent

Table for equivalence from final CGPA grade to percentage of marks for comparison form conventional marks system.

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Table 2

Final Grade	Equivalent percentage of marks
0 .	90% and more
A+	80% to less than 90%
A	70% to less than 80%
B+	60% to less than 70%
В	50% to less than 60%
С	45% to less than 50%
Р	40% to less than 45%
F	less than 40%

c) Grade Report

A copy of the grade report shall be issued to each student at the end of the semester.

d) Transcript

A Transcript shall be issued to a student on successful completion of the programme.

e) withholding of Grade Report / Transcript/Grade Sheet

The grade Report /Transcript/Grade sheet of a student shall be withheld if he/she has not paid his/her dues, or if there is a case of indiscipline pending against him/her.

Interpretation clause

In case of any difficulty arising during the course of implementation of these ordinances or in case of any unforeseen circumstance, the interpretation / decision of the Vice-Chancellor shall be final.

Dean, Faculty of Science (Member)

Dean, Faculty of Agriculture (Member) Dean, Faculty of Education (Member)

Dean, Faculty of Commerce

(Member)

Dean, Faculty of Laws 119

(Member)

Dean, Faculty of Arts

(Convener)