Scheme of
M.Sc. Chemistry

SRI SAI UNIVERSITY
PALAMPUR (H.P.), INDIA

Course Structure

Course Code	Title of Course	Marks				Credits			
		Theory	Practical	Internal Assessment	Total	L	T	P	Total
SEMESTER-I									
CHE101	Inorganic Chemistry– I Group Theory & Non Aqueous Solvent	60	-	40	100	4	0	0	4
CHE102	Organic Chemistry – I Reaction Mechanism and Stereochemistry	60	-	40	100	4	0	0	4
CHE103	Physical Chemistry– I Spectroscopy & Kinetics	60	-	40	100	4	0	0	4
CHE104	Mathematics for Chemists & Application of Computer in Chemistry	60	-	40	100	4	0	0	4
CHE105	Inorganic Chemistry Practical – I	-	50	-	50	0	0	3	1.5
CHE106	Organic Chemistry Practical – I	-	50	-	50	0	0	3	1.5
CHE107	Physical Chemistry Practical – I	-	50	-	50	0	0	3	1.5
SEMESTER-II									
CHE201	Inorganic Chemistry– II Metal Ligand Bonding & Magnatochemistry	60	--	40	100	4	0	0	4
CHE202	Organic Chemistry – II Aromatic, Elimination and Pericyclic Reactions	60	--	40	100	4	0	0	4
CHE203	Physical Chemistry– II Thermodynamics & Electrochemistry	60		40	100	4	0	0	4
CHE204	Chemistry of Life & Environmental Chemistry	60	--	40	100	4	0	0	4
CHE205	Inorganic Chemistry Practical – II	--	50	--	50	0	0	3	1.5
CHE206	Organic Chemistry Practical – II	--	50	--	50	0	0	3	1.5
CHE207	Physical Chemistry Practical – II		50	- -	50	0	0	3	1.5
SEMESTER-III									
CHE301	Inorganic Chemistry– III Analytical & Nuclear chemistry	60	--	40	100	4	0	0	4
CHE302	Organic Chemistry – III Organic Spectroscopy and Photochemistry	60	--	40	100	4	0	0	4

CHE303	Physical Chemistry – III Statistical Thermodynamics and Basic Quantum Chemistry	60		40	100	4	0	0	4
*	Special Paper – I	60	--	40	100	4	0	0	4
CHE305	Inorganic Chemistry Practical – III	---	50	--	50	0	0	3	1.5
CHE306	Organic Chemistry Practical – III	---	50	--	50	0	0	3	1.5
CHE307	Physical Chemistry Practical – III	---	50	--	50	0	0	3	1.5
CHE500A	Project Seminar	---	---	-	50	0	0	4	2

SEMESTER-IV

CHE401	Techniques of chemical analysis	60	--	40	100	4	0	0	4
CHE402	Chemistry of Materials	60	--	40	100	4	0	0	4
**	Special Paper – II	60		40	100	4	0	0	4
**	Special Paper – III	60	--	40	100	4	0	0	4
CHE500B	Project	----	--	--	200	0	0	16	8

List of Special Papers

*Semester – III

Course Code	Title of Course	Marks				Credits			
		Theory	Practical	Internal Assessment	Total	L	T	P	Total
CHE304I	Inorganic Chemistry Special Theory – I Bioinorganic And Reaction Mechanism	60	--	40	100	4	0	0	4
CHE304O	Organic Chemistry Special Theory – I Natural Products	60	--	40	100	4	0	0	4
CHE304P	Physical Chemistry Special Theory – I Surface Chemistry & Advanced Electrochemistry	60	--	40	100	4	0	0	4

****Semester – IV**

CHE403I	Inorganic Chemistry Special Theory – II Advanced Organometallics	60	--	40	100	4	0	0	4
CHE404I	Inorganic Chemistry Special Theory – III Inorganic Spectroscopy	60	--	40	100	4	0	0	4
CHE403O	Organic Chemistry Special Theory – II Synthetic Strategies	60	--	40	100	4	0	0	4
CHE404O	Organic Chemistry Special Theory – III Medicinal Chemistry	60	--	40	100	4	0	0	4
CHE403P	Physical Chemistry Special Theory – II Advanced Quantum Chemistry	60	--	40	100	4	0	0	4
CHE404P	Physical Chemistry Special Theory – III Solid State Chemistry	60	--	40	100	4	0	0	4

Courses of Study: M.Sc. (Chemistry)

SEMESTER-I

Inorganic Chemistry - I
Group Theory & Non Aqueous Solvent

CHE101

L	T	P	Credit
4	0	0	4

UNIT-I

Group theory: The concept of group, Symmetry elements and symmetry operations, Assignment of point groups to Inorganic molecules, Some general rules for multiplications of symmetry operations, Multiplication tables for water and ammonia, Representations (matrices, matrix representations for C_{2V} and C_{3V} point groups irreducible representations), Character and character tables for C_{2V} and C_{3V} point groups. Applications of group theory to chemical bonding (hybrid orbitals for σ-bonding in different geometries and hybrid orbitals for π-bonding.Symmetries of molecular orbitals in BF_3, C_2H_4 and B_2H_6.

UNIT-II

Application of Group Theory in Vibrational Spectroscopy: A brief idea about Infrared and Raman scattering spectroscopy. Vibrational modes as basis of group representations w.r.t. SO_2, $POCl_3$, $PtCl_{42-}$ and RuO_4.Mutual exclusion principle, Classification of vibrational modes (i.e. stretching and angle deformation vibrations w.r.t. SO_2, $POCl_3$ and $PtCl_{42-}$.

UNIT-III

Non-Aqueous Solvents: Factors justifying the need of Non Aqueous solution Chemistry and failure of water as a Solvent. Solution chemistry of Sulphuric acid: Physical properties, Ionic self-dehydration in H_2SO_4, high electrical conductance in spite of high viscosity, Chemistry of H_2SO_4 as an acid, as an dehydrating agent, as an oxidizing agent, as an medium to carry out acid-base neutralization reaction and as a differentiating solvent. Liquid BrF_3: Physical properties, solubilities in BrF_3 , self-ionization, acid base neutralization reactions, solvolytic reactions and formation of transition metal fluorides. Chemistry of Molten salts as Non-Aqueous Solvents: Solvent properties, solution of metals, complex formation, Unreactivity of molten salts, Low temperature molten salts.

UNIT-IV

Inorganic Hydrides: Classification, preparation, bonding and their applications. Transition metal compounds with bonds to hydrogen, carbonyl hydrides and hydride anions. Classification, nomenclature, Wade's Rules, preparation, structure and bonding in boron hydrides (boranes),carboranes, metalloboranes and metallocarboranes.

UNIT-V

Organic Reagents in Inorganic Chemistry: Chelation, factors determining the stability of chelates (effect of ring size, oxidation state of the metal, coordination number of the metal); Use of the following reagents in analysis:

(a) Dimethylglyoxime (in analytical chemistry)
(b) EDTA (in analytical chemistry and chemotherapy)

(c) 8-Hydroxyquinoline (in analytical chemistry and chemotherapy)
(d) 1,10-Phenanthroline (in analytical chemistry and chemotherapy)
(e) Thiosemicarbazones (in analytical chemistry and chemotherapy)
(f) Dithiazone (in analytical chemistry and chemotherapy)

Books recommended:

1. *Chemical applications of Group Theory - F.A.Cotton*
2. *Inorganic Chemistry - Durrant and Durrant*
3. *Symmetry in Chemistry- Jaffe and Orchin*
4. *Non-aqueous solvents - H.Sisler*
5. *Non-aqueous solvents - T.C.Waddington*
6. *Non-aqueous solvents - Logowsky*
7. *Advanced Inorganic Chemistry:Cotton& Wilkinson,Vth Edn.*
8. *Concise course in Inorganic Chemistry- J.D.Lee*
9. *Nature of Chemical Bond - L. Pauling*
10. *Chemistry of Elements - Greenwood and Earnshaw*
11. *Inorganic Chemistry - T. Moeller*
12. *Inorganic Chemistry - J.E.Huheey 3rd Edn.*
13. *Topics in Current Chemistry (Inorganic/Bio-Chemistry)-Vol. 64*
14. *A Text Book of Quantitative Inorganic Analysis- A.I. Vogel*

SEMESTER-I

Organic Chemistry – I
Reaction Mechanism and Stereochemistry

CHE102

L	T	P	Credit
4	0	0	4

UNIT-I

Nature of Bonding in Organic Molecules: Delocalized Chemical Bonding: Kinds of molecules with delocalized bond, cross- conjugation, resonance, pπ-dπ bonding (ylides). aromaticity: other systems containing aromatic sextet, Aromatic systems with electron number other than six. Huckel rule, other aromatic compounds, hyperconjugation. Supramolecular chemistry: Introduction, Bonding other than covalent bond. Addition compounds, Crown ether complexes and Cryptands, Inclusion compounds, Cyclodextrins, Catenanes and Rotaxenes and their applications.

UNIT-II

Stereochemistry: Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity in acylic and cyclohexane systems. Steric strain due to unavoidable crowding. Elements of symmetry: chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, Optical activity due to chiral planes, Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape. Asymmetric Synthesis: Principle and categories with specific examples of asymmetric synthesis including newer methods involving enzymatic and catalytic reactions, enantio and diastereoselective synthesis. Stereoselective Reactions: Cyclopropanation, hydroboration, catalytic hydrogenation, and metal ammoni reduction, stereoselective synthesis of (-) ephedrine and (+) φ- ephedrine. Stereospecific Reactions : Elimination of 2,3- dibromobutane densyl chloride(1,2-diphenyl-1-chloroethane), SN^2 reactions at chiral carbon.

UNIT-III

Reaction Mechanism: Structure and Reactivity: Thermodynamic and kinetic requirements, Kinetic and Thermodynamic control, Hammonds postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates.

Effect of structure on reactivity: resonance and field effects, steric effect. Quantitative treatment: Hammett equation and linear free energy relationship, Substituent and reaction constants, Taft equation. Methods of determining reaction mechanism.

UNIT-IV

Aliphatic Nucleophilic Substitution: The SN_2, SN_1, mixed SN_1 and SN_2, SET mechanisms & SNi mechanism. The neighboring group mechanism, neighboring group participation by π and σ bonds, anchimeric assistance. Non-classical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements-Wagner-Meerwein, Pinacol-Pinacolone and Demjanov ring expansion and ring contraction. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Esterification of carboxylic acid, transesterification, transetherification and preparation of inorganic esters. Phase-transfer catalysis, and ultrasound, ambident nucleophile, regioselectivity.

UNIT-V

I. **Aliphatic Electrophilic Substitution:** Bimolecular mechanisms- SE2 and SEi. The SE1 mechanism, electrophilic substitution accompanied by double bond shifts, halogenation of aldehydes, ketones, acids and acyl halides. Effect of substrates, leaving group and the solvent system on reactivity. Aliphatic diazonium coupling, Acylation at aliphatic carbon, alkylation of alkene, Stork-enamine reactions.

II. **Free radical reactions:** Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighboring group assistance, Reactivity in aliphatic and aromatic substrates at a bridgehead and attacking radicals. Effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Gomberg Bachmann reaction, Sandmeyer reaction, Hoffmann -Loffler- Freytag reaction, Hunsdiecker reaction.

Books recommended:

1. *Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.*
2. *Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.*
3. *A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, 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, Benjamin.*
7. *Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic and Professional.*
8. *Pericyclic Reactions, S.M. Mukherji, Macmillan, India.*
9. *Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.*
10. *Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.*
11. *Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.*

SEMESTER-I

Physical Chemistry– I
Spectroscopy & Kinetics

CHE103

L	T	P	Credit
4	0	0	4

UNIT - I

Spectroscopy - I: Theory of nuclear magnetic resonance NMR phenomenon, the chemical shift and its measurement. The fine structure (spin - spin coupling). Factors influencing chemical - shift and spin - spin coupling. Non - first - order spectra. Relaxation phenomena in NMR: spin - spin and spin - lattice relaxation processes. Line -width and rate processes. The nuclear Overhauser effect.An introduction to Fourier Transform NMR (FTNMR).Theory of Electron Spin Resonance (ESR) phenomenon.Fine and hyperfine structure of ESR. Zero - field splitting of ESR signal. Mapping of charge density on molecule (McConnell relation). Mossbaur spectroscopy: a brief introduction (isomer - shift, quadrupole interaction and magnetic hyperfine interaction).

UNIT - II

Spectroscopy - II: Rotational and vibrational spectra. Moment of inertia and rotational spectra of rigid and non - rigid diatomic molecules. Vibrational excitation effect..Rotational spectra of symmetric - top molecules.Strak effect.Vibrational energy of diatomic molecules.Anharmonic oscillator, overtones and hot bands.Diatomic vibrator - rotator (P, Q and R - branches of diatomic vibrator - rotator). Rotational - vibrational spectra of symmetric - top molecules. RamanSpectroscopy: qualitative quantum theory of Raman scattering. Rotational Raman spectra of linear and symmetric - top molecules.Vibrational Raman spectra and mutual exclusion principle.

UNIT - III

Kinetics of complex reactions: Reversible / opposing reactions, consecutive / successive reactions, simultaneous side / parallel reactions, chain / free radical reactions viz. thermal (H_2 - Br_2) and photochemical H_2 - Cl_2) reactions. Rice - Herzfeld mechanism of dissociation of organic molecules viz. dissociation of ethane, decomposition of acetaldehyde as 3/2 or ½ order reactions. Kinetics of polymerization (molecular and free radical mechanisms).Reaction rates and chemical equilibrium, principle of microscopic reversibility, activation energy and activated complex.

UNIT - IV

Theories of reaction rates: The kinetic theory of collisions, transition state theory, comparison of collisions and transition state theories in simple gas reactions, steric factor, transmission -coefficient, steady - state hypothesis / transient phase theory, Lindmans theory of unimolecular reaction, the thermodynamic formulation of reaction rates.

UNIT - V

1. **Surface Reactions**: Mechanism of surface reactions, unimolecular and bimolecular surface reactions, Langmuir - Hinshelwood mechanism for gases only.
2. **Fast Reaction in aqueous solutions**: Study of fast reactions by Stopped flow method (Principle and Theory). Absolute rate theory applied to fast reactions.

Books recommended:

1. *Chemical Kinetics: K.J. Laidler*
2. *Kinetics and Mechanism of Reaction Rates: A.Frost and G. Pearson.*
3. *Modern Chemical Kinetics: H. Eyring*
4. *Theories of Reaction Rates: K.J. Laidler, H. Eyring and S. Glasston*
5. *Fast Reactions: J.N. Bradly*
6. *Fast Reactions in Solutions: Caldin*
7. *Basic Principles of Spectroscopy: R. Chang*
8. *NMR and Chemistry: J.W. Akit*
9. *Introduction to Molecular Spectroscopy: G.M. Barrow*
10. *Physical Chemistry: P.W. Atkins*
11. *Fundamentals of Molecular Spectroscopy: C.N. Banwell*

SEMESTER-I

Mathematics for Chemists & Application of Computer in Chemistry

CHE104

L	T	P	Credit
4	0	0	4

Mathematics for Chemists

UNIT - I

Cartesian coordinates: plane polar coordinates, spherical representation of functions, the complex plane, polar coordinates in trigonometric functions. Differential calculus: functions of single and several variables, partial derivatives, the total derivative, maxima and minima theorem, and simple examples related to chemistry. Vectors: representation and simple properties of vectors (addition and subtraction) vector addition by method of triangles, resolution of vectors. Scalar product of vector.Concept of normalization, orthogonality and complete set of unit vectors.

UNIT - II

Integral calculus: general and special methods of integration, geometric interpretation of integral, evaluation of definite and some standard integrals related to chemistry. The significance of 'exponential' equations. Differential equations: simple differential equations, separable variables, homogeneous equations, exact equations, linear equations, and equations of first and second order. Application to simple chemistry problems.

UNIT - III

Matrices and Determinants: Definition of matrix, types of matrices (row, column, null, square, diagonal). Matrix algebra: addition, subtraction, and multiplication by a number, matrix multiplication. Transpose and adjoint of matrix, elementary transformation, representation and applications to solutions of linear equations. Definition of determinant, and its properties, evaluation of determinants. Application to simple chemistry problems.

Application of Computer in Chemistry

UNIT - IV

Chemistry and FORTRAN Programming: Introductory FORTRAN concepts, character set, constant variables, data types, subscripted variables, and FORTRAN functions. FORTRAN expressions and naming FORTRAN programme, assignment statements, FORTRAN commands. Data transfer and program execution control: Introduction, format specification for READ and WRITE statements, format commands, control commands and transfer commands.

UNIT – V

Arrays and replitive computation: Introduction, arrays arrange storage, dimension statement, do comtruel, Nested do - loop continue statement, implied do. Sub - programme (functions and sub– routines): Introduction, sub programme, functions in FORTRAN, function arguments, subroutines, save variable function vs. subroutine programme. Global variables and file manipulation:Introduction, common statement, equivalence declaration, data command, block data subprogramme, declaration external, character expression and assignment, the open and closed statement, internal file, file 'input' and 'output'. Developing Linear Least - Squares fit programs in FORTRAN, as well as for involving simple formulae in organic, inorganic and physical chemistry.

Books recommended:

1. *Mathematical Preparation for Physical Chemistry: F. Daniel*
2. *Mathematical Methods for Science Students: G. Stephemen*
3. *Applied Mathematics for Physical Chemistry: T.R. Barrante*
4. *Fortran 77 & 90: V. Rajaraman*
5. *Computer in Chemistry: K.V. Raman*

SEMESTER-I

INORGANIC CHEMISTRY PRACTICAL – I

CHE105

L	T	P	Credit
0	0	3	1.5

1. **Volumetric Analysis:**

   (a) **Potassium iodate titrations**: Determination of iodide, hydrazine, antimony(III) and arsenic (III)

   (b) **Potassium bromate titrations**
   i) Determination of antimony (III) and arsenic (III) Direct Method)
   ii) Determination of aluminium, cobalt and zinc (by oxine method)

   (c) **EDTA titrations**
   i) Determination of copper, nickel, magnesium
   ii) Back titration
   iii) Alkalimetric titration
   iv) Titration of mixtures using masking and demasking agents
   v) Determination of hardness of water

2. **Commercial Analysis:**

   i) Determination of available chlorine in bleaching powder
   ii) Determination of Oxygen in hydrogen peroxide.
   iii) Determination of Phosphoric acid in commercial phosphoric acid.
   iv) Determination of Boric acid in borax.
   v) Determination of metals: copper in copper oxychloride and zinc in zinebfungicides.

3. Analysis of mixtures by gravimetric and volumetric methods from the mixture solutions:

1. Copper- Nickel
2. Copper-Magnesium
3. Copper-Zinc
4. Iron-Magnesium
5. Silver-Zinc
6. Copper-Nickel-Zinc
7. Fe(II)-Fe(III)

4. Green methods of Preparation of the following:

1. Bis(acetylacetonato)copper(II)
2. Tris(acetylacetonato)iron(III)
3. Tris(acetylacetonato)manganese(III)

Books recommended:

1. A text Book of Quantitative Inorganic Analysis: A.I.Vogal.
2. Applied Analytical Chemistry: Vermani.
3. Commercial Methods of Analysis: Shell & Biffen

SEMESTER-I

ORGANIC CHEMISTRY PRACTICAL – I

CHE106

L	T	P	Credit
0	0	3	1.5

Qualitative Analysis:

I. Separation, purification and identification of binary mixture of organic compounds by chemical tests,
II. Thin Layer Chromatography
III. Column Chromatography
IV. IR spectroscopy.

Organic Synthesis:

A. Acetylation: - Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography.
B. Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol.
C. Grignard reaction: Synthesis of triphenyl methanol from benzoic acid.
D. Aldol condensation: Dibenzal acetone from benzaldehyde.
E. Sandmeyer reaction: p-chlorotoluene from p-toluidine.
F. Acetoacetic ester condensation: Synthesis of ethyl-n-butylacetoacetate by A.E.E condensation.
G. Preparation of iodoform from acetone (Haloform reaction).
H. Preparation of polystyrene, anthranilic acid, fluorosceine-eosin, and methyl orange.

Books recommended:

1. *Experiments and Techniques in Organic Chemistry, D.Pasto, C. Johnson and M.Miller, Prentice Hall.*
2. *Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C.Heath.*
3. *Systematic Qualitative Organic Analysis, H.Middleton, Adward Arnold.*
4. *Handbook of Organic Analysis-Qualitative and Quantitative, H.Clark, Adward Arnold. 5. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.*

SEMESTER-I

PHYSICAL CHEMISTRY PRACTICAL – I

CHE107

L	T	P	Credit
0	0	3	1.5

1. **Refractive Index (RI) Measurements**: Refractive index (RI) measurements of puresolvents, analysis of mixtures of two miscible solvents, molar and atomic refraction determination, polarizability of liquids.

2. **Conductometric Measurements**: Determination of cell constant, limiting molar conductance of simple electrolytes in water, verification of Ostwald, dilution law for week acetic acid.

3. **Surface Tension Measurements**: Surface tension of pure solvents, analysis of mixtures of two miscible solvents, verification of Gibb's Thomson Rule of surface tension.

4. **Partition - Coefficient**: Determination of partition - coefficient for I_2 between water and CCl_4 and for benzoic acid between water and benzene.

5. **Adsorption Measurements**: Verification of Freundlich adsorption isotherm for I_2,acetic acid and oxalic acid on charcoal.

6. **Colloidal Solution**: Preparation of sol solution of arsenic sulphide and estimation offlocculation value for NaCl, KCl, $BaCl_2$, $AlCl_3$.

7. **Thermochemistry**: Determination of water equivalent of thermos flask, and estimation of heat of neutralization for strong acid strong base, weak acid strong base or vice -versa, heat of hydration and solution of salts.

8. **Kinetic Measurement**: Kinetics of Hydrolysis of methylacetate and ethylacetate in thepresence of HCl.

Books recommended:

1. *Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla*
2. *Experimental Physical Chemistry: V. Athawale and P. Mathur.*
3. *Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.*
4. *Practical in Physical Chemistry: P.S. Sindhu*

SEMESTER-II

Inorganic Chemistry-II
Metal Ligand Bonding & Magnatochemistry

CHE201

L	T	P	Credit
4	0	0	4

UNIT-I

Metal-Ligand Bonding-I: Recapitulation of Crystal Field Theory including splitting of d-orbitals in different environments, Factors affecting the magnitude of crystal field splitting, structural effects (ionic radii, Jahn-Teller effect), Thermodynamic effects of crystal field theory (ligation, hydration and lattice energy), Limitations of crystal field theory, Adjusted Crystal Field Theory (ACFT), Evidences for Metal-Ligand overlap in complexes, Molecular Orbital Theory for octahedral, tetrahedral and square planar complexes (excluding mathematical treatment)

UNIT-II

Atomic Spectroscopy: Energy levels in an atom, coupling of orbital angular momenta, coupling of spin angular momenta, spin orbit coupling, spin orbit coupling p^2 case, Determining the Ground State Terms-Hund's Rule, Hole formulation (derivation of the Term Symbol for a closed sub-shell, derivation of the terms for a d^2 configuration), Calculation of the number of the microstates.

UNIT-III

Electronic Spectra-I: Splitting of spectroscopic terms (S,P,D.F and G,H,I), d^1-d^9 systems in weak fields (excluding mathematics), strong field configurations, transitions from weak to strong crystal fields.

Electronic Spectra-II: Correlation diagrams (d^1-d^9) in O_h and $T_d$environments, spin-cross over in coordination compounds. Tanabe Sugano diagrams, Orgel diagrams, evaluation of B,C and β parameters.

UNIT-IV

Electronic Spectra - III (Electronic spectra of complex ions): Selection rules (Laporte, orbital and spin selection rules), band intensities, band widths, spectra in solids, spectra of aqueous solutions of d^1-d^9 ions in O_h and T_d environments, Evaluation of 10 D_q, Spectrochemical and Nephelauxetic series, charge- transfer spectra.

UNIT-V

Magnetochemistry: Origin of Magnetic moment, factors determining paramagnetism, application of magnetochemistry in co-ordination chemistry (spin only moment, Russell Saunder's coupling, quenching of orbital angular moment, orbital contribution to a magnetic moment) in spin free and spin paired octahedral and tetrahedral complexes. Magnetic susceptibility(diamagnetic, paramagnetic), magnetic moments from magnetic susceptibilities, Van Vlecks formula for magnetic susceptibility, temperature dependence of magnetic susceptibility.

Books recommended:

1 *Advanced Inorganic Chemistry - Cotton and Wilkinson*

2 *Coordination Chemistry- Experimental Methods - K.Burger*

3 *Theoretical Inorganic Chemistry - Day and Selbin*

4 *Magnetochemistry - R.L.Carlin*

5 *Comprehensive Coordination Chemistry - Wilkinson, Gillars and McCleverty.*

6 *Inorganic Electronic Spectroscopy - A.B.P.Lever*

7 *Concise Inorganic Chemistry - J.D.Lee*

8 *Introduction to Ligand Fields - B.N.Figgis*

9 *Physical Methods in Inorganic Chemistry-R.S.Drago*

10 *Introduction to Magnetochemistry - A.Earnshaw, Academic Press.*

SEMESTER-II

Organic Chemistry-II
Aromatic, Elimination and Pericyclic Reactions

CHE202

L	T	P	Credit
4	0	0	4

UNIT - I

(A) **Aromatic Electrophilic Substitution**: Arenium ion mechanism, orientation and reactivity, energy profile diagrams, The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles, Diazonium coupling, Vilsmeir reaction, Scholl reaction, Amination reaction, Fries rearrangement, Reversal of Friedel Craft alkylation, Decarboxylation of aromatic acids.

(B) **Aromatic Nucleophilic Substitution**: SNAr, SN^1, benzyne and SRN^1 mechanism. Reactivity,effect of substrate structure, leaving group and attacking nucleophile, Von Richter, Sommelet-Hauser, and Smiles rearrangements, Ullman reaction, Ziegler alkylation, Schiemann reaction.

UNIT-II

Common Organic Reactions and Their Mechanisms: Perkin condensation, Michael reaction, Robinson annulation, Diekmann reaction, Stobbe condensation, Mannich reaction, Knoevenagel condensation, Benzoin condensation, Witting reaction, Hydroboration, Hydrocarboxylation, Ester hydrolysis, Epoxidation.

UNIT- III

Reagents in Organic Synthesis: Synthesis and applications of BF_3, NBS, Diazomethane, Lead tetra-acetate, Osmium tetraoxide, Woodward Prevorst hydroxylation reagent, $LiAlH_4$, Grignard reagent, organozinc and organolithium reagent.

UNIT-IV

Elimination Reactions: Discussion of E_1, E_2, E_1cB and E_2C Mechanisms and orientation, Reactivity: Effects of substrate structures, attacking base, leaving group and medium. Cis elimination, elimination in cyclic systems, eclipsing effects, Pyrolytic eliminations, cleavage of quaternary ammonium hydroxides, Fragmentations: γ-Amino and γ-hydroxy halides, decarboxylation of β-hydroxy carboxlic acid and β-lactones.

UNIT-V

Pericyclic Reaction: Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5 hexatrienes and allyl system. Classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions: conrotatory and disrotatory motions, 4n and 4n+2 and allyl systems. Cycloadditions- antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and chelotropic reactions. Sigmatropic rearrangements-Suprafacial and Antarafacial shifts of H, sigmatropic shifts involving carbon moieties, Claisen, Cope and aza-Cope rearrangements, Ene reaction.

Books recommended:

1. *Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.*
2. *Advanced Organic Chemistry, F.A. Carey and R.J. Sundberg, Plenum.*

3. *A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, 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, Benjamin.*
7. *Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, Blackie Academic and Professional.*
8. *Pericyclic Reactions, S.M. Mukherji, Macmillan, India.*
9. *Reaction Mechanism in Organic Chemistry, S.M. Mukherji and S.P. Singh, Macmillan.*
10. *Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.*

SEMESTER-II

Physical Chemistry-II
Thermodynamics & Electrochemistry

CHE203

L	T	P	Credit
4	0	0	4

UNIT – I

Brief resume of law of thermodynamics. Gibb's and Helmholtz free energy functions and their significance. Partial molal quantities. Partial molal free energy and its variation with temperature and pressure. Determination of partial molar volume. Thermodynamic criteria for the feasibility of the process in terms of entropy change, internal energy change, enthalpy and free energy (Gibb's and Helmholtz) change. Gibb's and Helmholtz equation and its utility in thermodynamics of cell reaction. Maxwell's relations, Joule-Thomson effect

UNIT – II

Chemical potential in case of ideal gases. Thermodynamics of ideal solutions. Fugacity and activity and their variation with temperature and pressure. Graphical method for the determination of fugacity. Chemical equilibrium constant and its temperature dependence. Law of chemical equilibrium and its application.

UNIT – III

Clausius and Clapeyron equation and its application for the determination of colligative properties (depression in freezing point, elevation in boiling point and relative lowering of vapour pressure). Determination of molecular weight of non – volatile solutes from colligative properties. Relationship between relative lowering of vapour pressure and osmotic pressure. Van't Hoff equation for dilute solutions and its application.

UNIT – IV

Nernst heat theorem and third law of thermodynamics and its application. Thermodynamic derivation of phase rule and its application to two component systems. Distribution law, its thermodynamic derivation and application. Zeroth law of thermodynamics. Basic principles of non – equilibrium thermodynamics:

UNIT –V

Electrochemistry: Electrochemical equilibrium, Nernst equation, Ionic conduction: non – ideal behaviour of electrolytic solutions. Electrolytical potential. Derivation of Debye – Huckel Limiting Law. Extended Debye – Huckel Law. Structure of solutions. Detailed treatment of ion – solvent interactions (ion solvation), solvation number. Energy conduction. Ion – ion interactions (ion – association). Bjerrum's theory of ion – association.

Books Recommended:

1. Thermodynamics for Chemists: S. Glasstone
2. Physical Chemistry: G.M. Barrow
3. Non – equilibrium Thermodynamics: C. Kalidas
4. Non – equilibrium Thermodynamics: I. Prigogene
5. Electrochemistry: S. Glasstone
6. Electrochemistry: P.H. Reiger
7. Thermodynamics; R.C. Srivastava, S.K. Saha and A.K. Jain
8. Modern Electrochemistry Vol. I: J.O'M Bockris and A.K.N. Reddy

SEMESTER-II

Chemistry of Life & Environmental Chemistry

CHE204

L	T	P	Credit
4	0	0	4

UNIT-I

Cell structure and function: Overview of metabolic processes (catabolic and anabolic), energy transfer processes, role and significance of ATP (the biological energy currency). Introductory idea of metabolism of proteins and lipids, biosynthesis of proteins and glycerides.

UNIT-II

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

UNIT-III

Environmental Chemistry: Atmosphere, environmental segments, composition of the atmosphere, earth's radiation balance, particulates, ions and radicals and their formation, chemical and photochemical reactions in the atmosphere, air pollution, oxides of C,N,S and their effects, acid-rain, smog formation, Green house effects (global warming and ozone depletion, air pollution controls and introduction to analytical methods for monitoring air pollution.

UNIT-IV

Hydrosphere: Chemical composition of water bodies-lakes, streams, rivers, sea etc, hydrological cycle, complexation in natural and waste water and microbially mediated redox reactions. Water pollution-inorganic, organic, pesticides, industrial and radioactive materials, oil spills and oil pollutants, eutrophication, acid-mine drainage, waste water treatment, domestic waste water (aerobic and anaerobic treatment), and industrial waste water treatment.

UNIT-V

Water quality parameters and standards: Analytical methods for measuring DO, BOD, COD, fluoride, oils and grease and metals (As, Cd, Hg, Pb, Zn,Cu,Cr), Biochemical effects of As, Cd, Hg, Pb, Cr, CN and pesticides. Lithosphere: Soil composition, micro and macro nutrients, soil pollution-fertilizers, pesticides.

Books recommended:

1. *Principles of Biochemistry -A.L.Lehringer*
2. *Introduction to Chemistry of Life-H.J.DeBay*
3. *Outlines of Biochemistry-Conn and Stumpf*
4. *Environmental Chemistry-A.K.De*
5. *Environmental Chemistry-Manaham*
6. *Environmental Pollution Analysis-Khopkar*

SEMESTER-II

INORGANIC CHEMISTRY PRACTICAL –II

CHE205

L	T	P	Credit
0	0	3	1.5

Preparation of the following compounds and a study of the important properties viz. Molar conductance, magnetic sussceptibility, electronic and infrared spectra.

1. Stannic iodide
2. Bis(acetylacetonate) oxovanadium (IV)
3. Tris (acetylacetonate) siliconchloride.
4. Mercuration of phenol.
5. Hexa ammine nickel (II) chloride.
6. Pyridine perchromate.

INSTRUMENTAL ANALYSIS:

(A) **Conductometric Titrations**:

i) Differential behaviour of acetic acid to determine the relative acid strength of various acids and basic strength of various bases.

ii) Strong acid-strong base titration in acetic acid.

(B) **Potentiometric Titrations**.

1. Neutralisation reactions:
   - i) Sodium hydroxide-hydrolchloric acid.
   - ii) Sodium hydroxide-Boric acid
   - iii) Acetic acid and hydrochloric acid-sodium hydroxide.

2. Oxidation-Reduction Reactions.
   - i) Ferrous-dichromate
   - ii) Ferrous-Ceric
   - iii) Iodine-Thiosulphate

3. Precipitation Reactions:
   - i) Silver nitrate-sodium halides.

4. Complexation Reactions
   - i) Potassium cyanide-silver nitrate.

(C) **Colorimetric Analysis**:

1. Verification of Beer's law for $KMNO_4$, $K_2Cr_2O_7$ solutions and determination of the conc. of $KMNO_4$ $K_2Cr_2O_7$ in the given solution.
2. Colorimetric determination of Iron (III) with potassium thiocyanate reagent or o-Phenanthroline method.
3. Determination of traces of manganese (in steel samples) colorometrically byoxidation to permanganic acid with potassium periodate.

4. Spectrophotometric determination of pK value of an indicator (acid dissociation constt. of methyl red)

(D) **pH metric –titrations**

1. Copper and cactechol
2. Copper and salicylic acid
3. Acid base titrations
4. Mixtures of acids with a base

(E) **Polarography:**

1. Determination of half wave potentials of cadmium ion in potassium chloride solution
2. Determination of half wave potentials of zinc and manganous ions in potassium
3. Determination of cadmium in solution
4. Investigation of the influence of dissolved oxygen.

(F) **Amperometric Titrations:**

1. Zinc with EDTA
2. Lead vs. chromate
3. Nickel as isoquilnoline thiocynate

(G) **Flame Photometry:**

1) Determination of sodium
2) Determination of potassium
3) Determination of calcium

(H) **Miscellaneous:**

1. Determination of stability constants of complexes.
2. Determination of magnetic susceptibility of complexes
3. Estimation of periodate, iodate and bromate in the same solution.
4. Determination of bromide and chloride in the same solution.
5. Analysis of a solution containing chloride and iodide.

Books recommended:

1. *A Text Book of Quantitative Inorganic Analysis- A.I. Vogel*
2. *Chemistry Experiments for Instrumental Methods:- D.T. Sawyer, W.R. Heinemanand J.M. Beebe.*
3. *Inorganic Synthesis- R.A. Rowe and M.M. Jones (1957)5, 113 - 116.*

SEMESTER-II

ORGANIC CHEMISTRY PRACTICAL –II

CHE206

L	T	P	Credit
0	0	3	1.5

(A) **Extraction of Organic Compounds from Natural Sources**: Isolation of Caffeine from tea leaves, casein from milk (the students are required to try some typical colour reactions of proteins), lactose from milk (purity of sugar should be checked by TLC and PC and Rf value reported). lycopene from tomatoes and β- carotene from carrots.

(B) **Paper Chromatography**: Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of Rf values.

(C) **Spectroscopy**:
Identification of some organic compounds by the analysis of their spectral data (UV, IR, PMR, CMR and MS)

- Multistep
- Synthesis of Vacor
- Synthesis of Indigo
- Synthesis of p- nitro aniline

Books recommended:

1. *Experiments and Techniques in Organic Chemistry, D.Pasto, C. Johnson and M.Miller, Prentice Hall.*
2. *Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C.Heath.*
3. *Systematic Qualitative Organic Analysis, H.Middleton, Adward Arnold.*
4. *Handbook of Organic Analysis-Qualitative and Quantitative, H.Clark, Adward Arnold.*
5. *Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.*

SEMESTER-II

PHYSICAL CHEMISTRY PRACTICAL –II

CHE207

L	T	P	Credit
0	0	3	1.5

1. **Viscosity Measurements**: Verification of the Jones - Dole equation, determination of viscosity A and B - coefficients for simple electrolytes in water and in aqueous mixtures of organic solvents.

2. **Conductometric Measurements**: Kinetics of saponification of ethylacetate by NaOH. Solubility of sparingly soluble salts.

3. **Potentiometric Titration**: Titration of HCl with NaOH, determination of dissociation constant of acetic acid and phosphoric acid. Oxidation - reduction titration (ferrous ammonium sulphate with $KMnO_4$ and $K_2Cr_2O_7$).

4. **Flamephotometric Measurements**: Establishing the calibration plots for Na^+ and K^+ ions and determination of their concentration in the given solution at ppm level.

5. **Determination of Molar Mass**: Cryoscopic and Rasts's methods. Determination of molar mass of polymer by viscosity measurement.

6. **Colometery Measurements**: Determination of composition ferric ions – salicylicacid complex using Job's method.

7. **Polarimetry Measurements**: Determination of specific and molecular rotation, percentage of tow optically active substances, kinetics of acid catalysed inversion of cane sugar, comparison of strengths of two acids.

Books recommended:

1. *Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla*
2. *Experimental Physical Chemistry: V. Athawale and P. Mathur.*
3. *Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.*
4. *Practical in Physical Chemistry: P.S. Sindhu*
5. *Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla*

SEMESTER-III

Inorganic Chemistry-III
Analytical & Nuclear chemistry

CHE301

L	T	P	Credit
4	0	0	4

UNIT-I

Metal π Complexes: Preparation, reactions, structures and bonding in carbonyl, nitrosyl, phosphine and related complexes, structural evidences from vibrational spectra, bonding and important reactions of metal carbonyls. Structure and bonding in metal cyanides, stabilization of unusual oxidation states of transition metals.

UNIT-II

Introductory Analytical Chemistry: Data Analysis- Types and sources of errors, propagation of errors, detection and minimization of various types of errors. Accuracy and precision, average and standard deviation, variance, its analysis and confidence interval, tests of significance (F-test, t-test and paired t-test), criteria for the rejection of analytical data (4d rule, 2.5d rule, Q-test, average deviation and standard deviation), least-square analysis.

Food and Drug Analysis- General methods for proximate and mineral analysis in food (moisture, ash, crude fiber, nitrogen (proteins) and minerals (iron, calcium, potassium, sodium and phosphorus). Discussion of official (pharmacopea) methods for the determination of following drugs as such: (i) Analgin/oxyphenbutazone, (ii) chloramphenicol and related nitro compounds, (iii) chloroquinine, (iv) phenyl butazone, (v) salicylic acid and (vi) sulphonamides.

UNIT-III

Photoelectron Spectroscopy: Basic principle, photoionization process, ionization energies, Koopman's theorem, ESCA, photoelectron spectra of simple molecules, (N_2, O_2 and F_2)
Photoelectron spectra for the isoelectronic sequence Ne, HF, H_2O, NH_3 and CH_4, chemical information from ESCA, Auger electron spectroscopy - basic idea.

UNIT-IV

Lanthanides and Actinides:- Spectral and magnetic properties, comparison of Inner transition and transition metals, Transuranium elements (formation and colour of ions in aqueous solution),uses of lanthanide compounds as shift reagents, periodicity of translawrencium elements.

UNIT-V

Nuclear Chemistry: Nuclear binding energy and stability, nuclear models (nuclear shell model and collective model). Nuclear reactions: types of reactions, nuclear cross-sections, Q-value. Natural and artificial radioactivity, radioactive decay and equilibrium, Nuclear fission-fission product and fission yields, Nuclear fusion.

Radioactive techniques: Tracer technique, (neutron activation analysis), Counting techniques such as G.M. Ionization and proportional counters.

Books recommended:

1. *Advanced Inorganic Chemistry - Cotton and Wilkinson*
2. *Fundamentals of Analytical Chemistry - Skoog and West*
3. *Quantitative Inorganic Analysis - Vogel*
4. *Chemistry of the Elements - Greenwood and Earnshaw*
5. *Nuclear Chemistry-U.C.Dash*
6. *Nuclear Chemistry - B.G.Harvey*
7. *Nuclear Chemistry - Arnikar*
8. *Techniques in Inorganic Chemistry Vol. II (Nuclear Chemistry-Johnson and Others).*
9. *Modern Aspects of Inorganic Chemistry-H.J.Emeleus and A.G.Sharpe*
10. *Inorganic Chemistry, 4^{th} Edition, - J.E.Huheey, E.A.Keiter and R.L.Keiter.*
11. *Analytical Chemistry-G.D.Christian*
12. *Chemical Structure and Bonding- Dekock and Gray*
13. *The Organometallic Chemistry of Transition metals: R.H. Crabtree.*
14. *Electronic absorption spectroscopy and related techniques: D.N. Sathyanarayan*

SEMESTER-III

Organic Chemistry-III
Organic Spectroscopy and Photochemistry

CHE302

L	T	P	Credit
4	0	0	4

UNIT-I

Spectroscopy:

(A) **Ultra Violet and Visible Spectroscopy**: Electronic transitions (185-800 nm), Beer- Lambert Law, Effect of solvent on electronic transitions, Ultra Violet bands of carbonylcompounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules forconjugated dienes and carbonyl compounds, Ultra- Violet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.Applications of UV- visible spectroscopy in organicchemistry.

(B) **Infrared Spectroscopy**: Instrumentation and sample handling, Characteristic vibrational frequencies of common organic compounds. Effect of hydrogen bonding and solvent effect onvibrational frequencies, overtones, combination bands and Fermi resonance.Introduction toRaman spectroscopy.Applications of IR and Raman Spectroscopy in organic chemistry.

UNIT-II

Nuclear Magnetic Resonance (NMR) Spectroscopy: General introduction, chemical shift, spin-spin interaction, shielding mechanism, chemical shift values and correlation of protons present in different groups in organic compounds. chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, four and five nuclei, virtual coupling. Stereochemistry, hindered rotation, Karplus-relationship of coupling constant with dihedral angle. Simplification of complex spectra-nuclear magnetic double resonance, spin tickling, INDOR, contact shift reagents, solvent effects. Fourier transform technique, Nuclear Overhauser Effect (NOE). Introduction to resonance of other nuclei -F, P, Principle and introduction to C^{13} NMR, 2-D and 3-D NMR, Applications of NMR in organic chemistry.

UNIT-III

Mass Spectrometry: Introduction, ion production—EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, and ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, Molecular ion peak, Meta-stable peak, McLafferty rearrangement. Nitrogen Rule.High-resolution mass spectrometry.Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.Introduction to negative ion Mass spectrometry, TOF-MALDI. Problems based upon IR, UV, NMR and mass spectroscopy.

UNIT- IV

Photochemistry - I: Introduction and Basic principles of photochemistry. Interaction ofelectromagnetic radiations with matter. Types of excitations, fate of excited molecules, quantum yield, transfer of excitation energy, actinometry. Photochemistry of alkenes: cis-trans isomerization, dimerization of alkenes, photochemistry of conjugated olefins, photo-oxidation of alkenes and polyenes Photochemistry of Aromatic compounds: Isomerization, addition and substitution, photo-reduction of aromatic hydrocarbons.

UNIT- V

Photochemistry - II: Photochemistry of Carbonyl compounds: Norrish Type I and II, Intermolecular and Intramolecular hydrogen abstraction, Paterno-Buchi reaction, α and β- cleavage reactions of cyclic and acyclic carbonyl compounds, Formation of oxetane and cyclobutane from α, β unsaturated ketones, Photo-reduction of carbonyl compounds, Photo-rearrangement of enones, dienones, epoxyketones, Photo Fries rearrangement.

Books recommended:

1. *Practical NMR Spectroscopy, M.L. Martin, J.J. Delpeuch and G.J.Martin, Heyden*
2. *Spectrometric Identification of Organic Compounds, R. M. Silverstein, G.C.Bassler and T.C.Morrill, John Wiley.*
3. *Introduction to NMR Spectroscopy, R.J. Abraham, J. Fisher and P. Loftus, Wiley.*
4. *Application of Spectroscopy of Organic Compounds, J.R. Dyer, Prentice Hall.*
5. *Spectroscopic Methods in Organic Chemistry, D.H. Williams,I. Fleming, Tata McGraw-Hill.*
6. *Organic spectroscopy by Jagmohan*
7. *Organic spectroscopy by W. Kemp.*
8. *Fundamentals of Photochemistry, K.K.Rohtagi - Mukherji, Wiley-Eastern.*
9. *Essentials of Molecular Photochemistry, A. Gilbert and J.Baggot, Blackwell Scientific Publication.*
10. *Molecular Photochemistry, N.J. Turro, W.A. Benjamin.*
11. *Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill.*
12. *Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson.*
13. *Organic Photochemistry, J. Coxon and B. Halton, Cambridge University Press.*
14. *Organic Photochemistry Vol.I, II, III. Ed. Orville L. Chapman.*
15. *Organic Photochemistry, Ed. Robert O. Kan.*

SEMESTER-III

Physical Chemistry-III

Statistical Thermodynamics and Basic Quantum Chemistry

CHE303

L	T	P	Credit
4	0	0	4

Statistical Thermodynamics

UNIT – I

Basic Terminology: probability, phase space, micro and macro states, thermodynamic probability, statistical weight, assembly, ensemble, probability considerations and chemistry. The most probable distribution: Maxwell-Boltzmann distribution, Thermodynamic properties from statistical Thermodynamics, The Partition Function for monoatomic gas, State functions in terms of partition function, separating partition function: the nuclear and electronic partition function, for molecules, electronic and vibrational partition function,

UNIT – II

Diatomic molecules: Rotations, Polyatomic molecules: Rotations, The partition function of a system, Thermodynamic properties of molecules from partition function: Total energy, entropy, Helmholtz free energy, pressure, heat content, heat capacity and Gibb's free energy, equilibrium constant and partition function, Heat capacity of crystals and statistical thermodynamics, quantum statistics: The Bose- Einstein statistics and Fermi-Dirac Statistics.

Basic Quantum Chemistry

UNIT – III

Operators in quantum mechanics. Eignvalues and eignfunctions. Hermitian operator and its application. Postulates of quantum mechanics. Angularmomentum of a one – particle system, and its commutative relations. Schreodinger wave equatuion and its formulation as an eignvalue problem. The uncertainty principle.

UNIT – IV

Quantum mechanical treatment of translational motion of a particle, particle in one and three dimensional boxes, harmonic – oscillator, rotational motion of a particle: particle on a ring, particle on a sphere, rigid rotator and hydrogen atom. Graphical presentation of orbitals (s, p and d), radial and angular probability distribution plots.

UNIT – V

Photochemistry: Photophysical processes of electronically excited molecules. Intensity distribution in the electronic vibrational species. Franck – Condon principle a quantum – mechanical treatment. Excited state dipole moment and acidity constant. Dissociation and pre – dissociation of diatomic molecules. Energy transfer from electronically excited molecules: Stern – Volmer mechanism only. Photophysical pathways: fluorescence, phosphorescence, E-typeand P- type delayed fluorescence. Kinetic treatment of excimer and exciplex formation.

Books Recommended:

1. Physical Chemistry: D.W. Ball
2. Theoretical Chemistry by S. Glasston
3. Statistical Chemistry by I. Prigogine
4. Quantum Chemistry An Introduction: H.L. Strauss
5. Introductory Quantum Chemistry: A.K. Chandra
6. Quantum Chemistry: A. Mcquarrie
7. Quantum Chemistry: I.N. Levine

SEMESTER-III

Inorganic Chemistry Special Theory – I
(Bioinorganic Chemistry and Reaction Mechanism)

CHE304I

L	T	P	Credit
4	0	0	4

UNIT-I

(a) **Metalloporphyrins**: (ref. Books No. 1,5,6): Porphyrins and their salient features, characteristic absorption spectrum of porphyrins, chlorophyll (structure and its role in photosynthesis). Transport of Iron in microorganisms (sidrophores), types of siderophores (catecholate and Hydroxamato siderophores).

(b) **Metalloenzymes**: (Ref. Book No. 1,2): Definitions: Apoenzyme, Coenzyme, Metalloenzyme, structure and functions of carbonic anhydrase A & B, carboxy peptidases.

UNIT-II

Oxygen Carriers: (Ref. Book No. 1,8):

a) **Natural oxygen carriers**: Structure of hemoglobin and myoglobin, Bohr effect, Models for cooperative interaction in hemoglobin, oxygen Transport in human body (-perutz machanism), Cyanide poisoning and its remedy. Non-heme protiens (Hemerythrin &Hemocyanin).

b) **Synthetic oxygen carriers**: Oxygen molecule and its reduction products, model compounds for oxygen carrier (Vaska's Iridium cjomplex, cobalt complexes with dimethyl glyoxime and schiff base ligands).

UNIT-III

Transport and storage of metals: **(Ref. Books No. 1,2)** The transport mechanism, transport of alkali and alkaline earth metals, ionophores, transport by neutral macrocycles and anionic carriers, sodium/potassium pump, transport and storage of Iron (Transferrin & Ferritin).

Inorganic compounds as therapeutic Agents (Ref. Books N. 1,4,8):- Introduction chelation therapy, synthetic metal chelates as antimicrobial agents, antiarthritis drugs, antitumor, anticancer drugs (Platinum complexes), Lithium and mental health.

UNIT-IV

Supramolecular Chemistry (Ref. Book 9): Introduction, Some important concepts, Introduction to Recognition, information and complementarity, Principles of molecular receptor designs, Spherical recognition (cryptates of metal cations) Tetrahedral recognition by macrotricycliccryptands, Recognition of ammonium ions, Recognition of neutral molecules and anionic substrates (anionic coordination)

UNIT-V

Inorganic Reactions and Mechanism: Substitution reactions in octahedral complexes, acid hydrolysis reactions, base hydrolysis and anation reactions, substitution reaction, reactions occurring without rupture of metal-ligand bond. Substitution reactions of square planar complexes.Theories of trans-effect, labile and inert complexes.Mechanism of redox reactions.

Books recommended:

1. *The Inorganic Chemistry of Biological processes - M.N.Hughes.*
2. *Bio Inorganic Chemistry - Robert Wittay*
3. *Advanced Inorganic Chemistry (4th Edn) - Cotton and Wilkinson.*
4. *Topics in current chemistry (Inorganic Biochemistry) vol. 64 (1976) - Davison and Coworkers.*
5. *An Introduction to Biochemcial Reaction Mechanism - James N.Lowe and Lloyalt Ingraham.*
6. *General Biochemistry - Fruton J.S. and Simmonds S.*
7. *Plant Physiology - Robeert N.Devtin.*
8. *Inorganic chemistry - James E. Huheey.*
9. *Supramolecular Chemistry (Concepts and Perspectives) - Jean Marie Lehn(VCH-1995).*
10. *Advanced Inorganic Chemistry- Cotton and Wilkinson*
11. *Inorganic Reaction Mechanism - Edberg*
12. *Inorganic Reaction Mechanism - Basoloavd Pearsor*

SEMESTER-III

Organic Chemistry Special Theory – I

(NATURAL PRODUCTS)

CHE304O

L	T	P	Credit
4	0	0	4

UNIT-I

Terpenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure determination, biosynthesis and synthesis of the following representative molecules: Monoterpenoids: Citral, geraniol (acyclic), α-terpeneol, menthol (monocyclic). Sesquiterpenoids: Farnesol (acyclic), zingiberene (monocyclic), santonin (bicyclic), Diterpenoids: Phytol and abietic acid.

UNIT- II

Carotenoids and Xanthophylls: General methods of structure determination of Carotenes: β-carotene, α- carotene, γ- carotene, lycopene and vitamin A. Xanthophylls: Spirilloxanthin, Capsorubin, Fucoxanthin. Carotenoid acids (Apocarotenoids): Bixin and Crocetin. Bio synthesis of carotenoids

UNIT-III

Alkaloids: Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, synthesis and biosynthesis of the following: Ephedrine, Coniine, Nicotine, Atropine, Quinine and Morphine.

UNIT-IV

Steroids: Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Androsterone, Testosterone, Estrone, Progestrone. Biosynthesis of steroids

UNIT-V

Plant Pigments: Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Anthocyanins (Cyanin and pelargonidin), polyphenols: Flavones (chrysin), Flavonols(quercitin) and isoflavones (daidzein) coumarin, Quinones (lapachol), Hirsutidin. Biosynthesis of flavonoids: Acetate pathway and Shikimic acid pathway.

Books recommended:

1. *Natural Products- Chemistry and Biological Significance, J. Mann, R.S. Davidson, J. B. Hobbs,D.V. Banthrope and J. B. Harborne, Longman, Essex.*
2. *Organic Chemistry Vol. II, I.L. Finar, ELBS.*
3. *Stereo selective synthesis- A Practical Approach, M. Nogradi, VCH.*
4. *Rodd's Chemistry of Carbon Compounds, Ed. S. Coffey, Elsevier.*
5. *Chemistry, Biological and Pharmacological Properties of Medicinal Plants From the Americas, Ed.Kurt Hostettmann, M.P. Gupta and A. Marston, Harwood Academic Publishers.*
6. *Introduction to Flavonoids, B.A.Bohm, Harwood Academic Publishers.*
7. *New Trends in Natural Product Chemistry, Atta-ur-Rahman M. I. Choudhary, Harwood Academic Publishers.*
8. *Insecticides of Natural Origin, Sukh Dev, Harwood Academic Publishers.*

SEMESTER-III

Physical Chemistry Special Theory – I
(Surface Chemistry & Advanced Electrochemistry)

CHE304P

L	T	P	Credit
4	0	0	4

UNIT –I

Adsorption at solid – gas interface: Concept of ideal and non – ideal adsorption. Heat of adsorption. Types of adsorption isotherms. Single – layer adsorption – Langmuir adsorption isotherm and its derivation. Multilayer adsorption – B.E.T. theory and its kinetic derivation. Application of BET theory in its determination of surface area of the solid. Catalytic activities at surfaces: adsorption and catalysis.

UNIT –II

Adsorption at solid – liquid interface: Gibbs adsorption equation. Isotherms of concentration and temperature change for the adsorption in solutions. Chromatographic adsorption: column chromatography and its theory. Theory of chromatography involving one solute and several solutes.

UNIT –III

Solution and Interfacial Behaviour of Surfactants: Definition and classification of surfactants. Solution properties of surfactants: micelle and reverse micelle formation, critical micelle concentration (CMC), dependence of CMC on chain length of the surfactant, micelle shape andsize. Thermodynamics of micelle formation, hydrophobic effect (a qualitative view only). Aggregation at high surfactant concentration (a qualitative aspect). to micelles. Surface tension and detergent., Practical application of surfactants.

UNIT –IV

Electrochemistry: Mechanism of electrolytic conductance, relaxation and electrophoretic effects, Debye – Huckel – Onsager (DHO) equation and its validity in aqueous and non aqueous solutions. Deviations from the Onsager equation, conductance ratio and Onsager equation. Dispersion of conductance at high frequencies (Debye – Falkenhagen effect). Conductance with high potential gradients (Wien effect). Activity and activity coefficient, forms of activity coefficients, activities of electrolytes and mean ion activity coefficient. The Debye – Huckel Limiting law. Electrokinetic phenomena: Electrical double layer and its structure (Stern's theory), Electroosmosis, Streaming potential, Electrophoresis, Influence of ions on electrokinetic phenomena (Qualitative insight).

UNIT –V

Chemistry of nano – materials: Definition and historical perspective. Effect of nanoscience and nanotechnology in various fields. Synthesis of nanoparticles by chemical routs and their caracterization techniques. Properties of nanostructured material: optical, magnetic and chemical properties. An overview of applied chemistry of nanometerials.

Books Recommended:

1. Physical Chemistry of Surfaces: A.W. Admson
2. Adsorption from Solutions: J.J. Kipling
3. Micelles (Theoretical and Applied Aspects): Y. Moroi
4. Foundation of Colloid Science Vol. I and II: R.J. Hunter
5. Physical Chemistry: P.W. Atkins
6. Frontiers in Applied Chemistry: A.K. Biswas
7. Introduction to nanotechnology: Charles P.Poole, Jr. Frank, J. Owens: Wiley India

SEMESTER-III

INORGANIC CHEMISTRY PRACTICAL –III

CHE305

L	T	P	Credit
0	0	3	1.5

1. Analysis of the given sample (Ores)/Both Qualitative and Quantitative Dolomite, Pyrolusite, Galena.
2. Analysis of the given alloys: Coin, Gunmetal, Brass and Bronze.
3. To prepare a pure and dry sample of the following compounds:

1. Potassium tris(oxalato)aluminate(III)
2. Sodium hexa(nitro)cobaltate(III)
3. Potassium tris(oxalato)cobaltate(III)
4. Hexa(ammine)cobalt (III)chloride
5. Tetrapyridine copper(II)persulphate
6. Dinitrotetrapyridine nickel(II)
7. Lead tetraacetate
8. Mercury (tetraisothiocyanato)cobaltate(II).

and characterize them by the following techniques:

i) Elemental analysis
ii) Molar conductance values
iii) I.R. Spectral interpretation
iv) Thermal analysis
v) UV-Visible Spectra

Books recommended:

1. A Text Book of Qualitative Inorganic Analysis - A.I. Vogel

SEMESTER-III

ORGANIC CHEMISTRY PRACTICAL –III

CHE306

L	T	P	Credit
0	0	3	1.5

A. **Quantitative Analysis:**

Determination of the percentage/ number of hydroxyl groups in an organic compound by acetylation method. Estimation of amines/ phenols using bromate –

bromide solution/ acetylation method. Determination of iodine and sponification values of an oil sample. Determination of DO, COD and BOD of water sample.

B. **Multistep Synthesis:**

Cannizzaro reaction: 4-chlorobenzaldehyde as substrate.

Benzilic Acid Rearrangement: Benzaldehyde → Benzoin→ Benzil→ Benzilic acid. **Hofmann bromamide Rearrangement** : Phthalic anhydride → Phthalimide→ Anthranilic acid

BeckmannRearrangement: Benzene→Benzophenone→BenzophenoneOxime→Benzanilide.

Skraup Synthesis: Preparation of quinoline from aniline.

Synthesis using Phase Transfer Catalysis: Alkylation of diethyl malonate or ethyl acetoacetate and an alkyl halide.

Books recommended:

1. *Experiments and Techniques in Organic Chemistry, D.Pasto, C. Johnson and M.Miller, Prentice Hall.*
2. *Macroscale and Microscale Organic Experiments, K.L. Williamson, D.C.Heath.*
3. *Systematic Qualitative Organic Analysis, H.Middleton, Adward Arnold.*
4. *Handbook of Organic Analysis-Qualitative and Quantitative, H.Clark,Adward Arnold.*
5. *Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.*

SEMESTER-III

PHYSICAL CHEMISTRY PRACTICAL –III

CHE307

L	T	P	Credit
0	0	3	1.5

1. **Solubility Measurements**:Heat of solution of electrolytes by solubility measurements.

2. **Heat of transfer Measurements**: Heat of transfer for benzoic acid between benzene and water and I_2 between CCl_4 and water.

3. **Conductometric Measurements**: Precipitation titration ($AgNO_3$ - KCl), acid - base neutralization titration, determination of relative strength of acids in the given mixtures, solubility of sparingly soluble salt.

4. **Construction of Phase Diagram**: Phase diagram for liquids, (benzene and methanol, --) and phase diagram for solids, (benzoic acid and cinnamic acid, benzoic acid and naphthalene and acetamide and salicylic acid).

5. **Colorimetric Measurements**: Verification of Beer - Lambert's law for aqueous solutions of $KMnO_4$, $K_2Cr_2O_7$ and $CuSO_4$ and construction of calibration plot to estimate the unknown concentration.
6. **Kinetic Measurement**: Saponification of ethylacetate by NaOH solution.

Books recommended:

1. *Senior Practical Physical Chemistry: B.D. Khosla, V.C. Garg and A. Khosla*
2. *Experimental Physical Chemistry: V. Athawale and P. Mathur.*
3. *Practical Physical Chemistry: B. Vishwanathan and P.S. Raghavan.*
4. *Practical in Physical Chemistry: P.S. Sindhu*

SEMESTER-III

Seminar

CHE-308

L	T	P	Credit
0	0	4	2

Every candidate will have to deliver a seminar of 15-30 minutes duration on a topic related to his/her project work hich will be chosen by him / her in consultation with the teacher of the department. The seminar will be delivered before the students and teachers of the department. A three member committee (one coordinator and two teachers of the department of different branches) duly approved by the departmental council will be constituted to evaluate the seminar. The following factors will be taken into consideration while evaluating the candidate.

(i) Expression

(ii) Presentation

(iii) Depth of the subject matter and answers to the questions.

SEMESTER-IV

(TECHNIQUES OF CHEMICAL ANALYSIS)

CHE401

L	T	P	Credit
4	0	0	4

UNIT-I

Spectrophotometry: i) Introduction, fundamental laws of photometry, the electromagnetic spectrum and spectrochemical methods, UV/Visible instrumentation, absorption spectra, Beer-Lambert's Law, deviation from Beer-Lambert's Beer's Law. ii) Photometric Titrations:- Simultaneous spectrophotometric determination, differential spectrophotometry, titration curves and applications to quantitative analysis. iii) Molecular Fluorescence Spectroscopy:- Theory, relaxation processes, relationship between excitation spectra and florescence spectra, florescencent species, effect of concentration on florescence intensity, instrumentation and application of florescence methods.

UNIT-II

Atomic Spectroscopy: Theory of flame photometer, intensities of spectral lines, selection of optimal working conditions, applications of flame photometry to quantitative analysis. The Theory of Atomic Absorption Spectroscopy (AAS), Origin of atomic spectra, line width effects in atomic absorption, instrumentation and its application, Atomic emission spectroscopy (AES) and the detailed description of the techniques of inductively coupled plasma AES (ICP-AES) and its instrumentation. Chemical and spectral interferences encountered in both techniques and how to overcome them.

UNIT-III

Electroanalytical Methods:

a) **Electrogravimetric methods**:- i) Current-voltage relationship during electrolysis, operation of a cell at a fixed applied potential, costant current electrolysis, physical properties of electrolytic precipitates, chemical factors of importance in electrodeposition, anodic deposition. ii) Spontaneous electrogravimetric analysis (internal electrolysis), apparatus and applications. iii) Electrolytic method with and without potential control, apparatus and applications.

b) **Coulometric Methods**: i) Controlled potential Coulometry, instrumentation and applications. ii) Coulometric titrations, cell for coulometric titrations, applications of coulometric titrations (neutralization, precipitation, andcomplex formation titrations), comparison of coulometric and volumetric titrations.

UNIT-IV

Polarographic Methods: General introduction: Theoretical measurements of classical polarography, polarographic measurements, polarograms, interpretation of polarographic waves, equation for polarographic waves, half-wave potential, effect of complex formation on polarographic waves, dropping mercury electrode (advantages and limitations), current variation with a dropping electrode, polarographic diffusion current, the ilkovic equation, effect of capillary characterization on diffusion current, diffusion coefficient temperature, kinetic and catalytic current, polarograms for mixtures of reactants, anodic waves and mixed anodic and cathodic waves, current maxima and its suppression, residual current, supporting electrolytes, oxygen waves, instrumentation and applications to inorganic and organic analysis.

UNIT-V

(a) ***Thermogravimatric* analysis**: Introduction, Factors affecting thermogravimetric curves, instrumentation, applications to inorganic compounds (analysis of binary mixtures i.e. Ca and Mg, TG curves of calcium oxalate, determination of Ca, Sr & Ba ions in the mixture, drying of sodium carbonate, analysis of clays and soils, decomposition of potassium hydrogen phthalate, oxidation of nickel sulphide, determination of titanium content of non-stoichiometric sample of titanium carbide).

(b) **Differential thermal analysis**: Introduction, Factors effecting DTA curves, instrumentation, applications, to inorganic compounds (thermal decomposition of mixtures of lanthanum-cerium and praseodymium oxalate, DTA curves for $CuSO_4.5H_2O$, sulphur, detection of organic contamination in ammonium nitrate, thermal decomposition for different magnesium carbonate samples, determination of uncalcined gypsum in plaster of paris.

Books recommended:

1. *Instrumental methods of analysis.-H.H.Willard, LL.Marritt and J.A.Dean*
2. *Fundamental of analytical Chemistry -D.A.Skoog & D.M.West*
3. *Basic concepts of analytical Chemistry-S.M.Khopkar*
4. *Instrumental Methods of Chemcial Analysis-G.K.Ewring*
5. *Quantitative Inorganic Analysis-A.I.Vogel*
6. *Ion Exchange-AellFerish*
7. *Modern Polarographic Methods in Analytical Chemistry -A.M.Bond*
8. *Thermal Methods of Analysis-W.W. Wandlandt.*
9. *D.A.Skoog, F.J.Holler and T.E.Nieman, Principles of Instrumental analysis, 5th Edition, Saunder's college Pub. 1998.*

SEMESTER-IV

(Chemistry of Materials)

CHE402

L	T	P	Credit
4	0	0	4

UNIT-I

Multiphase Materials :

Ferrous alloys , Fe-C phase transformations in ferrous alloys , stainless steels, non-ferrous alloys , properties of ferrous and non-ferrous alloys and their applications.

UNIT-II

Glasses , Polymers, Ceramics and Composites :

Glasses : Introduction , manufacturing , types and applications. Polymes : Molecular shape, structure and configuration , crystallinity , stress-strain behaviour, Thermal behavior, polymer types and their applications , conducting and ferro- electric polymers. Ceramics and refractories : Introduction , classification , characteristics, properties , some important high refractory materials and their applications. Composites : Introduction , constituents , classification , some industrially Important composites, failure modes and applications.

UNIT-III

Nanomaterials and Fullerenes :

Nanomaterials: Introduction , carbon nanotubes – their synthesis , properties and applications. Nanotechnology in diagnostic applications . Semiconductor quantum dots – synthesis, electronic structure and correlation of properties with size and their applications.

Fullerenes : Introduction , synthesis and purification , conductivity and superconductivity in doped fullerenes , chemistry of fullerenes . Properties – optical properties, ferromagnetism and some unusual properties of fullerenes.

UNIT-IV

Liquid Crystals :

Introduction , classification , chemical constitution and liquid crystalline behavior, molecular ordering in different mesophases , identification of liquid crystals , polymeric liquid crystals , applications of liquid crystals in displays and in thermography.

UNIT-V

Superconductors :

Introduction , types , properties , preparations , structure of superconductors and applications of low temperature and high temperature superconductivity.

Books recommended:

1. Solid State Physics, N. W. Ashcroft and N. D. Mermin, Saunders College Ed. 1976.

2. Principles of the Solid State, H.V. Keer, New Age International Publishers, Ed. 1993.

3. Materials Science, J.C. Anderson and K.D. Leaver, ELBS, Ed. 1971.

4. Handbook of Liquid Crystals, H. Kelker, R. Hatz and C. Schumann, Chemie Verlag, Ed. 1980.

5. Solid State Physics, J. S. Blakemore, Cambridge University Press, 1985.

6. Introduction to Material Science and Engineering, Y. W. Chung, CRC Press, Ed. 2007.

SEMESTER-IV

Inorganic Chemistry Special Theory – II
(ADVANCED ORGANOMETALLICS)

CHE403I

L	T	P	Credit
4	0	0	4

UNIT-I

Organometallic Compounds of transition elements: Types of ligands and their classifications in organometallic compounds , 16 and 18 electron rule and its limitations. Hapto-nomenclature, synthesis, structure and bonding aspects of following organometallic compounds with carbon- π donor ligands

a) Two electron donor (olefin and acetylenic complexes of transition metals)
b) Three electron donor (π-allyl complexes of transition metals)
c) Four electron donor (butadiene and cyclobutadiene complexes of transition metals)
d) Five electron donor (cyclopentadienyl complexes of transition metals - metallocenes with special emphasis to ferrocenes)
e) Six electron donor [Benzene (arene) complex]

Fluxional and dynamic equillibria in compounds such as η^2-olefin, η^3- allyl and dienyl complexes.

UNIT-II

Homogeneous Transition metal catalysis: General considerations, Reason for selecting transition metals in catalysis (bonding ability, ligand effects, variability of oxidation state and coordination number), basic concept of catalysis (molecular activation by coordination and addition), proximit y interaction (insertion/inter-ligand migration and elimination, rearrangement). Phase transfer catalysis. Homogeneous hydrogenation of unsaturated compounds (alkenes, alkynes, aldehydes and ketones).Asymmetric hydrogenation.

UNIT-III

Some important homogeneous catalytic reactions:- Ziegler Natta polymerization of ethylene and propylene, oligomerisation of alkenes by aluminumalkyl, Wackers acetaldehyde synthesis, hydroformylation of unsaturated compounds using cobalt and rhodium complexes, Monsanto acetic acid synthesis, carboxylation reactions of alkenes and alkynes using nickel carbonyl and palladium complexes. Carbonylation of alkynes (acetylene) using nickel carbonyls or Palladium complexes.

UNIT-IV

Metal-metal bonding in carbonyl and halide clusters:- Polyhedral model of metal clusters, effect of electronic configuration and coordination number, Structures of metal carbonyl clusters of three atoms $M_3(CO)_{12}$ (M=Fe, Ru & Os), Four metal atoms (tetrahedra) [$M_4(CO)_{12}$ {M= Co, Rh &Ir}] and octahedron of type $M_6(CO)_{16}$ [M= Co & Rh], and halide derivatives of Rhenium (III) triangles, metal carbonyls involving bridged-terminal exchange and scrambling of CO group.

Transition Metal-Carbon multiple bonded compounds:-Metal carbenes and carbynes (preparation, reactions, structure and bonding considerations). Biological applications and environmental aspects of organometallic compounds, Organometallic compounds in medicine, agriculture and industry.

UNIT-V

Stability of Coordination Compounds- Stability constants, stepwise formation constants,overall formation

constants, relationship between stepwise and overall formation constants, difference between thermodynamic and kinetic stability.

Determination of stability constants by:

(i) Spectrophotometric methods (Job's method, Mole ratio and slope ratio method).
(ii) Bjerrum's method
(iii) Leden's method
(iv) Polarographic method

Factors affecting the stability constants (with special reference to metal and ligand ions).

Books recommended:

1. *Principles of organometallic compounds – Powell*
2. *Organometallic chemistry (an Introduction) – Perkin and Pollar*
3. *Organometallic chemistry – Parison*
4. *Advanced Inorganic Chemistry - Cotton and Wilkinson*
5. *Organometallic Chemistry-R.C.Mehrotra*
6. *Organometallic compounds of Transition Metal-Crabtree*
7. *Chemistry of the Elements - Greenwood and Earnshaw*
8. *Inorganic Chemistry - J.E.Huheey*
9. *Homogeneous transition metal catalysis - Christopher Masters*
10. *Homogeneous Catalysis - Parshall*
11. *Principles and Application of HomogeneousCatalysis - Nakamura and Tsutsui*
12. *Progress in Inorganic Chemistry Vol. 15 - Lipard. (Transition metal clusters - R.B.King)*
13. *Organotransition metal chemistry by S.G.Davis, Pergamon press 1982.*
14. *Principles and applications of organotransition metal chemistry by Ccollmen and Hegden*

SEMESTER-IV

Inorganic Chemistry Special Theory – III
(INORGANIC SPECTROSCOPY)

CHE404I

L	T	P	Credit
4	0	0	4

UNIT-I

Infrared Spectroscopy: Theory of IR absorption, Types of vibrations, Observed number of modes of vibrations, Intensity of absorption bands, Theoretical group frequencies, Factors affecting group frequencies and band shapes (Physical state, Vibrational Coupling, Electrical effects, Resonance, Inductive effects, Ring strain) Vibrational-rotational fine-structure. Experimental method.Application of IR to the following:

i) Distinction between
   a) Ionic and coordinate anions such as NO_3^-, SO_4^{2-} and SCN^-
   b) Lattice and coordinated water.

ii) Mode of bonding of ligands such as urea, dimethylsulphoxide and hexamethylphosphoramide.

UNIT-II

Nuclear Magnetic Resonance Spectroscopy:- Introduction to Nuclear Magnetic Resonance, Chemical shift, Mechanism of electron shielding and factors contributing to the magnitude of chemical shift, Nuclear overhausser effect, Double resonance, Chemical exchange, Lanthanide shift reagents and NMR spectra of paramagnetic complexes. Experimental technique(CW and FT).

Stereochemical non-rigidity and fluxionality: Introduction, use of NMR in its detection, its presence in trigonal bipyramidal molecules(PF_5), Systems with coordination number six ($Ti(acac)_2Cl_2$, $Ti(acac)_2Br_2$, $Ta_2(OMe)_{10}$,).

UNIT-III

Nuclear Quadrupole Resonance Spectroscopy: Basic concepts of NQR (Nuclear electricquadrupole moment, Electric field gradient, Energy levels and NQR frequencies), Effect ofmagnetic field on spectra, Factors affecting the resonance signal (Line shape, position of resonance signal) Relationship between electric field gradient and molecular structure. Interpretation of NQR data, Structural information of the following: PCl_5, $TeCl_4$, Na^+GaCl_{4-}, BrCN, HIO_3 andHexahalometallates

UNIT-IV

Mossbauer Spectroscopy: Introduction, Principle, Conditions for Mössbauer Spectroscopy, parameters from Mössbauer Spectra, Isomer shift, Electric Quadrupole Interactions, Magnetic Interactions MB experiment, Application of MB spectroscopy in structural determination of the following:

i) High spin Fe (II) and Fe (III) halides FeF_2, $FeCl_2.2H_2O$, FeF_3, $FeCl_3.6H_2O$. Low spin Fe(II) and Fe(III) Complexes-Ferrocyanides, Ferricyanides, Prussian Blue.

ii) Iron carbonyls. $Fe(CO)_5$, $Fe_2(CO)_9$ and $Fe_3(CO)_{12}$

iii) Inorganic Sn(II) and Sn(IV) halides.

UNIT-V

Electron Spin Resonance Spectroscopy:-. Introduction, Similarities between ESR and NMR, Behaviour of a free electron in an external Magnetic Field, Basic Principle of an Electron Spin Resonance Spectrometer, Presentation of the spectrum, Hyperfine coupling in Isotropic Systems
(methyl, benzene and Naphthalene radicals). Factors affecting the magnitude of g-values. Zero field splitting and Kramer's Degeneracy, Line width in solid state ESR, Double resonance technique in e.s.r. (ENDOR) Experimental method. Applications of ESR to the following:

1. Bis-Salicylaldiimine - Copper –II
2. $CuSiF_6.6H_2O$ & $(NH_3)_5Co\text{-}O.Co(NH_3)_5$

Books recommended:

1. *Physical methods in Inorganic Chemistry - R.S.Drago.*
2. *Modern Optical methods of Analysis - Eugens D.Olsen*
3. *Infrared spectra of Inorganic and coordination compounds - Kazuo Nakamoto*
4. *Introduction to Chemistry -Donald L.Pavia and G.M.Lampman.*
5. *Fundamentals of Molecular Spectroscopy-C.N.Banwel*
6. *Spectroscopy in Inorganic Chemistry - Rao & Ferraro Vol I & II*
7. *Advances in Inorganic and Radiation Chemistry Vol 6 & 8.*
8. *Quarterly reviews Vol 11 (1957)*
9. *Progress in Inorganic Chemistry Vol 8*
10. *Organic Spectroscopy-W. Kemp*

SEMESTER-IV

Organic Chemistry Special Theory – II
(SYNTHETIC STRATEGIES)

CHE403O

L	T	P	Credit
4	0	0	4

UNIT-I

Organic Reagents: Reagents in organic synthesis: Willkinson catalyst, Lithium dialkyl cuprates (Gilman's reagents), Lithium diisopropylamide (LDA),1,3-Dithiane (Umpolung) Dicyclohexylcarbobiimide (DCC), and Trimethylsilyliodide, DDQ, SeO_2, Baker yeast, Tri-n-butyltinhydride, Nickel tetracarbonyl, Trimethylchlorosilane.

UNIT-II

Oxidations: Introduction, Different oxidative process. Aromatiztion of six membered ring, dehydrogenation yielding C-C double bond, Oxidation of alcohols, Oxidation involving C-C double bond, Oxidative cleavage of ketones, aldehydes and alcohols, double bonds and aromatic rings, Ozonolysis, Oxidative decarboxylation, Bisdecarboxylation, Oxidation of methylene to carbonyl, Oxidation of olefines to aldehydes and ketones.

UNIT -III

Reductions: Introduction, Different reductive processes. Reduction of carbonyl to methylene in aldehydes and ketones, Reduction of nitro compounds and oximes, Reductive coupling, bimolecular reduction of aldehydes or ketones to alkenes, metal hydride reduction, acyloin ester condensation, Cannizzaro reaction, Tishchenko reaction, Willgerodt reaction .

UNIT-IV

Rearrangements: General mechanistic considerations-nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements: Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Backmann, Hofmann, Curtius, Schmidt, Benzidine, BaeyerVilliger, Shapiro reaction, Witting rearrangement and Stevens rearrangement.

UNIT-V

Disconnection Approach: An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity cyclisation reactions, amine synthesis. Protecting Groups: Principle of protection of alcohol, amine, carbonyl and carboxyl groups.One Group C-C Disconnection: Alcohols and carbonyl compounds, regioselectivity. Alkene synthesis, use of acetylenes in organic synthesis.

Books recommended:

1. *Designing Organic Synthesis, S. Warren, Wiley.*
2. *Organic Synthesis- Concept, Methods and Starting Materials, J. Fuhrhop and G. Penzillin, VerlageVCH.*
3. *Some Modern Methods of Organic Synthesis, W. Carruthers, Cambridge Univ. Press.*
4. *Modern Synthetic Reactions, H.O. House, W. A. Benjamin.*
5. *Advanced Organic Chemistry-Reactions Mechanisms and Structure, J. March, Wiley.*

6. *Principles of Organic Synthesis, R. Norman and J.M. Coxon, Blakie Academic and Professional.*
7. *Advanced Organic Chemistry Part-B, F.A. Carey and R. J. Sundburg, Plenum Press.*
8. *Organomettalic Chemistry-A Unified Approach, R.C. Mehrotra, A. Singh.*

SEMESTER-IV

Organic Chemistry Special Theory – III
(MEDICINAL CHEMISTRY)

CHE404O

L	T	P	Credit
4	0	0	4

UNIT-I

Drug Design: Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism bio-isosterism, spatial considerations. Theories of drug activity: occupancy theory, rate theory, induced fit theory. Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors.Elementary treatment of drug receptor interactions. Physico-Chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Free-Wilson analysis, Hansch analysis relationships between Free-Wilson and Hansch analysis.

UNIT-II

Pharmacokinetics and Pharmacodynamics: Pharmacokinetics: Introduction to drug absorption, disposition, elimination using pharmacokinetics. Important pharmacokinetic parameters in defining drug disposition and in therapeutics. Mention of uses of pharmacokinetics in drug development process.

Pharmacodynamics: Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, sulphonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation. Significance of drug metabolism in medicinal chemistry.

UNIT-III

Antibiotics and Antiinfective Drugs: Antibiotics: Structure, SAR and biological action of antibiotics. Examples: penicillin: penicillin G, penicillin V, ampicillin, amoxycillin, chloramphenicol, cephalosporin, tetracycline and streptomycin.

Sufonanmides: Structure, SAR and mode of action of sulfonamides, sulfonamide inhibition and probable mechanisms of bacterial resistance to sulfonamides. Examples: sulfodiazine, sulfofurazole, acetyl sulfafurazole, Sulfagnanidine, Phthalylsulfo acetamide, Mafenide. Sulphonamide related compounds Dapsone. Local antiinfective drugs: Introduction and general mode of action. Examples: sulphonamides, furazolidone, nalidixic acid, ciprofloxacin, norfloxacin, chloroquin and primaquin

UNIT-IV

Psychoactive Drugs: Introduction, neurotransmitters, CNS depressants and stimulants. SAR and Mode of actions. Central Nervous System Depressant: General anaesthetics.

Sedatives & Hypnotics: Barbiturates and Benzodiazepines.

Anticonvulsants: Barbiturates, Oxazolidinediones, Succinimides, Phenacemide and Benzodiazepines.

Psycotropic Drugs: The neuroleptics (Phenothiazines and butyrophenones), antidepressants (Monoamine oxidases inhibitors and Tricyclic antidepressants) and anti-anxiety agents (Benzodiazepines).

Central Nervous System Stimulants: Strychnine, Purines, Phenylethylamine, analeptics, Indole ethylamine derivatives,

UNIT-V

Therapeutic Agents, SAR and Their mode of Actions: Antineoplastic Agents: Cancer chemotherapy, role of alkylating agents and antimetabolites in treatment of cancer. Mention of carcinolytic antiobiotics and mitotic inhibitors. Biological action of mechlorethamine, cyclophosphamide, melphalan, uracil, and 6-mercaptopurine.

Cardiovascular Drugs: Antihypertensive and hypotensive drugs, antiarrrhythemic agents, vasopressor drug Direct acting arteriolar dilators. Biological action of methyldopa, propranolol hydrochloride, amyl nitrate, sorbitrate, verapamil, Atenolol.

Antihistaminic agents: Ethylene diamine derivatives, amino alkyl ether analogues, cyclic basic. **Antifertility agents**: General antifertility agents.

Diuretics: Mercurial diuretic, Non mercurial diuretics (Thiazides, carbonic-anhydrase inhibitors, xanthine derivatives, pyrimidine diuretics and osmotic diureteics

Books recommended:

1. *An Introduction to Medicinal Chemistry, Graham L. Patrick.*
2. *Medicinal Chemistry: Principles and Practice Edited by F.D. King.*
3. *Textbook of Organic Medicinal and Pharmaceutical Chemistry, Edited by Charles O. Wilson, Ole Gisvold, Robert F. Doerge.*
4. *Introduction to Medicinal Chemistry, Alex Gringuage.*
5. *Principles of Medicinal Chemistry, William O. Foye, Thomas L. Lemice and David A. Williams.*
6. *Introduction to Drug Design, S.S. Pandeya and J. R. Dimmock, New Age International.*
7. *Burger's Medicinal Chemistry and Drug Discovery, Vol-1 (Chapter-9 and Ch-14), Ed. M.E. Wolff, John Wiley.*
8. *Goodman and Gilman's Pharmacological Basis of Therapeutics, Mc Graw-Hill.*
9. *The Organic Chemistry of Drug Design and Drug Action, R.B. Silverman, Academic Press.*
10. *Strategies for Organic Drug Synthesis and Design, D. Lednicer, John Wiley.*

SEMESTER-IV

Physical Chemistry Special Theory – II
(ADVANCED QUANTUM CHEMISTRY)

CHE403P

L	T	P	Credit
4	0	0	4

UNIT - I

Time – independent perturbation theory for non – degenerate states (first order correction to energy and wave function), and its application to particle in a one – dimensional box, ground state helium atom (without spin consideration) and perturbed harmonic – oscillator. Variational method: theory and application to ground state hydrogen and helium atoms and one – imensional oscillator.

UNIT - II

Theory of time – dependent quantum approximation technique. Fermi Golden Rule. Radiation – Matter interaction (induced emission and absorption of radiation). Einstein's transition probabilities. Determination of selection rules in respect of rigid rotation and harmonic – oscillator approximation.

UNIT - III

Quantum – mechanical of multielectron atoms: Hartree self – consistent method. Hartree – Fock self – Consistent (HFSCF) method. Rootham's method. Correlation energy (CE) and configuration interaction (CI). Koopmann's theorm. Basic idea of Density Functionla Theory (DFT): Kohn – Sham equation.

UNIT – VI

Quantum – mechanical treatment of diatomic molecules: The Born Oppenheimer approximation and its formulation. The valence – bond treatment of a hydrogen molecule. Heitler – London treatment and ionic contribution. Molecular Orbital Theory (MOT) of H2+. MOT with configuration interaction (CI). Hybridization (sp, sp2 and sp3) from a quantum – mechnical view –point.

UNIT – V

Quantum – mechanical treatment of Π - electron systems. The Π - electron approximation . Free electron molecular orbital (FEMO) method and its application to polyenes. The Huckel –Molecular Orbital Theory (HMOT) for conjugated hydrocarbons and cyclic conjugated systems.

Huckel calculations for ethylene, allyl systems, cyclobutadiene and benzene. Calculation of electron density, charge distribution and bond orders.

Books Recommended:

1. Quantum Chemistry An Introduction: H.L. Strauss
2. ntroductory Quantum Chemistry: A.K. Chandra
3. Quantum Chemistry: D.A. McQuarri
4. Quantum Chemistry: I.N. Levine
5. Molecular Quantum Mechanics: P.W. Atkins
6. Elementary Quantum Chemistry: F.L. Pilar
7. Introductory Quantum Chemistry: S.R. LaPaglia
8. Fundamental Quantum Chemistry: T.E. Peacock

SEMESTER-IV

Physical Chemistry Special Theory – III
(SOLID STATE CHEMISTRY)

CHE404P

L	T	P	Credit
4	0	0	4

UNIT - I

X- ray diffraction: Indexing of powder and crystal photographs. Determination of Bravais lattice, point group and space group. Determination of space group with examples. Electron diffraction: The scattering of electron by gases (Wierl equation), visual method, radial distribution method and applications.

UNIT - II

Bonding in crystals: Ionic crystals, lattice energy of ionic crystals, metallic crystals. Band theory. Imperfections: Point defects (Schottky and Frankel defects). Thermodynamic derivation of these defects. Theories of Bonding: Free electro theory; quantum approach, Fermi – Dirac statistics. Zone theory: quantum approach, allowed energy zones , Brillioun zones, k – space, Fermi surfaces and density states.

UNIT - III

Properties of crystals: Electrical properties of metals; conductors and non – conductors, conductivity in pure metals. Hall effect. Thermal properties: Theories of specific heat. Electrical properties of semiconductors: Band theory, intrinsic and extrinsic semiconductors. Electrons and holes. Temperature dependence and mobility of charge carriers. Optical properties: Absorption spectrum, photoconductivity, photovoltaic effect and luminescence. Refraction Birefringence and color centre. Dielectric properties: Piezoelectricity, Ferro electricity, Ionic conductivity and electric breakdown.

UNIT – IV

Superconductivity: Experimental survey, occurrence of superconductivity, destruction of superconductivity by magnetic fields (Meissner effect). Thermodynamic effects of superconducting species (entropy, thermal conductivity and energy gap). Quantum tunnling. Theoretical survey (thermodynamics of superconducting transition, London equation, coherence length). BCS theory of superconductivity.

UNIT - V

Solid State Reactions: General principles: experimental procedures, kinetics of solid state reactions, vapour phase transport methods, interaction or ion exchange reaction, electrochemical reduction methods, preparation of t5his films, growth of single crystal, high pressure and hypothetical method.

Books Recommended:

1. Introduction to Solids: Azaroff
2. Solid State Chemistry and its applications: West
3. Solid State Chemistry: Charkrabarty
4. Solid State Chemistry: N.B. Hannay
5. Solid State Physics: Kiittal

Polymer Science: P. Bhadur and N.V. Sastry

SEMESTER-IV

Project: MINOR PROJECT FOR ALL THREE SPECIALIZATIONS

CHE405

L	T	P	Credit
0	0	16	8

Every candidate will have to work on minor project on different topic which will be chosen by him / her in consultation with his/her supervisor. Which include Literature review, experimental works and discussions regarding their industrial and commercial applications. A three member committee (one coordinator and two teachers of the department of different branches) duly approved by the departmental council will be constituted to evaluate the project. The following factors will be taken into consideration while evaluating the candidate.

(i) Project Report

(ii) Presentation

(iii) Viva-Voce.