M. Sc Applied Chemistry

Detailed syllabi: M.Sc I Yr

Semester-I

S.No.	Paper	Name of course	Paper code	Contact Hours per week	Max marks		Total
					Sessionals	End Semester	
1.	Paper-I	Physical Chemistry-I	CY-511	03	30	70	100
2.	Paper-II	Physical Chemistry-II	CY-513	03	30	70	100
3.	Paper-III	Inorganic Chemistry-I	CY-515	03	30	70	100
4.	Paper-IV	Environmental and Solid State Chemistry	CY-517	03	30	70	100
5.	Paper-V	Organic Chemistry-I	CY-519	03	30	70	100
6.	Paper-VI	Organic Natural Products-I	CY-521	03	30	70	100
7.	Lab work	M.Sc. I Sem.Lab	CY-523P	18	90	210	300

Semester-II

S.No.	Paper	Name of course	Paper code	Contact Hours per week	Max marks		Total
					Sessionals	End Semester	-
1.	Paper-I	Physical Chemistry-III	CY-512	03	30	70	100
2.	Paper-II	Analytical Chemistry	CY-514	03	30	70	100
3.	Paper-III	Inorganic Chemistry-II	CY-516	03	30	70	100
4.	Paper-IV	Bio-inorganic Chemistry	CY-518	03	30	70	100
5.	Paper-V	Organic Chemistry-II	CY-520	03	30	70	100
6.	Paper-VI	Organic Natural Products-II	CY-522	03	30	70	100
7.	Lab work	M.Sc. II Sem Lab	CY-524P	18	90	210	300

Semester I

Paper-I (Physical Chemistry-I)) [CY-511]

- 1. Unifying Principles: Electromagnetic radiation, interaction of electromagnetic radiation with matter- absoption, emission, transmission, reflection, refraction, dispersion, polarization and scattering. Uncertainty relation and natural line with and natural line broadening, transition probability, results of the time dependent perturbation theory, transition moment, selection rules intensity of spectral lines, Born Oppenheimer approximation, rotational, vibrational and electronic energy levels.
- **2. Quantum Chemistry:** Wave particle duality, Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz, particle in a box the harmonic oscillator, the rigid rotor, the hydrogen atom.
- **3. Electronic Structure of Atoms:** Electronic configuration, Russell- Saunders terms and coupling schemes, Slater- Condon parameters, term separation energies of the pⁿ configuration, term separation energies for the dⁿ configurations, magnetic effects: spin-Orbit coupling and Zeeman splitting.
- **4. Electrochemistry:** Metal/Electrolyte interface: OHP and IHP, potential profile across double layer region, potential difference across electrified interface; Structure of the double layer: Helmholtz-Perrin, Gouy-Chapman, and Stern models, Butler-Volmer equation under near equilibrium and non-equilibrium conditions, exchange current density, Tafel plot, Polarizable and non-polarizable interfaces. Conductimetry: Ostwald dilution law, Debye-Huckel limiting law, Onsager equation.

Books Recommended:

- 1. P. W. Atkins, Physical Chemistry, Oxford University Press, New York.
- 2. S.Glasston, Physical Chemistry, Nostrand
- 3. Advance Physical Chemistry (Vol-1,2,3,4), K.L. Kapoor, Mac millan India
- 4. Puri, Sharma, Pathania, Advance Physical chemistry
- 5. Advance Physical Chemistry, Gurdeep Raj, Pragati Pakashan, Meerut.
- 6. J.O'M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Vol. 2, Plenum Press, New York.

Paper-II (Physical Chemistry-II)) [CY-513]

- 1. Chemical Kinetics: Kinetics of III order reaction, kinetics of parallel, opposing, consecutive and chain reactions, kinetics of unimolecular reactions, Lindeman theory, Collision and activated complex theory, comparison of results with Eyring and Arrhenius equation, Hinshelwood theory, RRKL theory, Kinetics of homogeneous catalyst, kinetics of enzyme catalyzed reaction.
- 2. Macromolecules: Polymer- definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization. Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures.
- **3.** Computer Science: Various number systems eg binary, decimal, hexadecimal, octadecimal numbers, Introduction and history of computer, various components of computers, classification of hardware, various operating systems, Central processor unit. Input devices. Storage devices preliminary information regarding programming in computer sciences and internet surfing and usages.
- **4. Symmetry and Group Theory:** Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups by matrices.

- 1. P. W. Atkins, Physical Chemistry, Oxford University Press, New York.
- 2. K. J. Laidler, Chemical Kinetics, Harper & Row, New York.
- 3. F.W. Billmayer, Jr., Text Book of Polymer Science, Wiley-Interscience, New York.
- 4. Puri, Sharma, Pathania, Advance Physical chemistry
- 5. Advance Physical Chemistry (Vol-1,2,3,4), K.L. Kapoor, Mac millan India
- 6. P.K. Bhattacharya: Group Theory & Its Chemical Applications
- 7. Group theory in Chemistry, Ramkrishnan etal
- 8. Computer, Fundamentals-P.K.Sinha

Paper-III (Inorganic Chemistry-I) [CY-515]

1. Chemistry of Non-Transitions elements:

General discussion on the properties of non-transition elements, preparation, properties and structure of boric acid, borates, boron nitrides, boro hydrides (diborane), carboranes, oxides and oxy acids of nitrogen, phosphorous, sulphur and chlorine, inter halogen compounds, poly halide ions, pseudo halogens, fluorocarbons and basic of noble gases, preparation, structure and bonding of noble gas compounds.

2. Chemistry of Transition Elements:

General characteristics, variable oxidation states, complex formation, color, magnetic and catalytic properties, comparative study of 4d & 5d transition elements with 3d analogues with respect to their ionic radii, oxidation states and magnetic properties.

3. General chemistry of "f" Block Elements:

Lanthanides and actinides, separation, oxidation states, magnetic and spectral properties, Lanthanides contraction

- 1. Inorganic chemistry: Cotton & Wilikinson
- 2. Advanced inorganic chemistry: J. D. Lee
- 3. Selected topics in Inorganic chemistry: W. U. Malik, G. D. Tuli and R. D. Madan.
- 4. Advanced inorganic chemistry vol I& II: Gurdeep Raj
- 5. Advanced inorganic chemistry: Cotton & Wilikinson, Wiley

Paper-IV(Environmental and Solid State Chemistry)[CY-517]

1. Environmental Chemistry

Inorganic Pollutants

- a. Aquatic pollution: water quality parameters viz. dissolved oxygen, biochemical oxygen demand, heavy metals Cl⁻, SO4²⁻, NO³⁻, PO4³⁻ contents.
- b. Soil pollution (including agricultural, viz. pesticides, fertilizers, plastics and metals), Waste treatment.
- c. Industrial pollution, viz. cement, sugar, distillery, drug, paper and pulp, thermal power plants, metallurgy.
- d. Domestic pollution viz. sewage, detergents, oil pollutants and its management
- 2. Solid state chemistry: Classification of solids, seven crystal systems, elements of symmetry in crystals, Space lattice and unit cell, Classification of solids on the basis of bond types; ionic solid, metallic solids, covalent solids, molecular solids. The packing of spheres, hcp, ccp, and bccp. Coordination number, radius ratio rules, calculation\ of limiting radius ratio values. Structures of NaCl, ZnS, CsCl, CaF₂, CdI₂, & rutile. Imperfection in crystals, stoichiometric non-stoichiometric defects, impurity, defects, semiconductors. Elementary study of liquid crystals.

- 1. Inorganic chemistry: Cotton & Wilikinson
- 2. Advanced inorganic chemistry: J. D. Lee
- 3. Selected topics in Inorganic chemistry: W. U. Malik, G. D. Tuli and R. D. Madan.
- 4. Advanced inorganic chemistry vol I& II: Gurdeep Raj
- 5. Advanced inorganic chemistry: Cotton & Wilkinson, Wiley
- 6. Environmental chemistry and pollution control: S.S. Dara.
- 7. Environmental chemistry: C. Baird, W.H. Freeman & Co. Newyork
- 8. Chemical pollution: A Global Overview: UNEP
- 9. Environmental chemistry: A.K. Day, New Age International Ltd.
- 10. Environmental chemistry: B.K. Sharma & H. Kaur, Goel Publishing House
- 11. Pollution Science: Pepper, Gebra & Brusseam, Academic Press.
- 12. Quantitative Inorganic Analysis, A.I. Vogel.
- 13. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
- 14. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard & J.S. Valentine, University Science Books

Paper-V(Organic Chemistry-I)[CY-519]

- 1. Nature of bondings in organic molecules: Delocalized chemical bonding-conjugation, cross conjugation, resonance, hyperconjugation, tautomerism, Aromaticity in benzenoids and non benzenoid compounds, Huckel rule, Homoaromatic and antiaromatic systems, steric hinderance, hydrogen bonding, Charge transfer complexes.
- **2. Stereochemistry:** Conformational analysis of acyclic systems and cycloalkanes (6-8 membered), Optical isomerism, Chirality, Chiral Synthesis, Geometrical isomerism in acyclic and cyclic, Condensed and bridged systems, methods of interconversion E to Z and vice-versa.
- **3. Substitution and elimination reactions:** S_N2 & S_N1 S_Ni change, solvent effect, competition b/w S_N2 & S_N1 mechanism, elimination reactions, E₁, E₂ and E₁CB mechanism, Hofmann elimination, cyclic elimination, Competition between elimination and substitution reactions
- **4. Reactive Intermediates:** Classical and non classical carbocation, carbanions, radicals, radical anions, radical cations, carbenes, arynes and nitrenes, general methods of generation, detection and reactivity of these intermediates, singlet oxygen, its generation and its reaction with organic compounds.
- **5. Named reactions:** Claisen condensation, Hofmann bromide degradation, Beckmann's rearrangement, Pinacole-Pinacolone rearrangement, Perkin, stobbe, Dieckmann condensation, Schmidt, Lossen, Curtius, Fries rearrangement, Reimer-Tiemann reaction, Reformatsky and Grignard reaction, Diels- alder reaction, Friedal Craft reaction, Witting reaction Hydroboration, Clemmenson, Wolf-Kishner, Meerwein, Pondorf-Varely and Birch reductions

- 1. Reactions and reagent in organic synthesis: O.P.Agarwal Goel Publishing House.
- 2. Stereochemistry of carbon compounds: Eliel, TMH Publishing Co. Ltd.
- 3. Synthetic organic chemistry: O.P.Agarwal Goel Publishing.
- 4. Mechanism in organic chemistry: Peter Syke
- 5. Advanced organic chemistry: Jerry March, Wiley
- 6. Synthetic reactions: House.

Paper-VI (Organic Natural Products-I)[CY-521]

- 1. **Alkaloids**: General methods for determining structure of alkaloid including Hofmann's exhaustive methylation method, Emde degradation, Von Braun's method for secondary and tertiary cyclic amines: Structure determination of following:
 - Pyridine or Piperidine group: Conine, Piperine, Ricinine., Pyrrolidine group Hygrine, Pyrrolidine and pyridine group Nicotine, Isoquinoline group Papaverine
- **2. Terpenoids:** Isolation, Isoprene rule, general methods of structure determination with particular emphasis on Acyclic monoterpenoids: Myrcene, and Citral; Monocyclic monoterpenoids: α-Terpineol, Carvone ; Bicyclic monoterpenoids: Camphor, Diterpenoid phytol, Acyclic sesqueterpenoids Farnnesol
- 3. **Purines:** Structure and synthesis of Uric acid. Synthesis of Adenine, Guanine, Caffeine, Threobromine, Theophylline and Xanthine.

- 1. Organic Chemistry: R.T. Morrison and R.N. Boyd P.H. Ltd.
- 2. Topics in Organic Chemistry: Fieser and Fieser, Reinhold.
- 3. Organic Chemistry: Vol. I & II: I.L.Finar, Elbs with Longmann Pub.

II Semester

Paper-I (Physical Chemistry-III)[CY-512]

- 1. Photochemistry: Introduction of photochemical phenomenon, laws of photochemistry, quantum yield and its experimental determination, Jablonski diagram, photosensitization and quenching, photochemical rate law, kinetics of photochemical reactions (formation of hydrogen chloride, hydrogen bromide, decomposition of acetaldehyde etc.), Photochemistry of stratospheric ozone, Lasers in photochemical reactions.
- 2. Surface Chemistry: Physisorption and chemisorption, adsorption isotherms, Langmuir and B. E. T. equation and significance in surface area determination, Study of adsorption kinetics (Lagergren equation, pseudo-second-order equation and Elovich model), Gibbs adsorption isotherm and its derivation, surface compositions, adsorption catalysis. Surface activity, surface active agents and their classification, micellisation, critical micelle concentration (CMC) thermodynamics of micellisation, factors affecting CMC.
- **3. Thermodynamics:** Brief resume of concept of laws of thermodynamics, entropy and entropy change, concept of free energy, Carnot cycle, Partial molar properties and their significance. Gibbs duhem equation, Fugacity: its concept and determination. Properties of ideal solutions; non-ideal systems-deviations (negative and positive) from ideal behaviour, excess functions for non-ideal solutions, calculations of partial molar quantities, determination of partial molar volume and partial molar enthalpy.

- 1. P. W. Atkins, Physical Chemistry, Oxford University Press, New York.
- 2. Advance Physical Chemistry (Vol-1,2,3,4), K.L. Kapoor, Mac millan India
- 3. Chemical Thermodynamics, S.M. Mukherjee and S.P. Singh, Vikas Publication, India
- 4. Themodynamics by R. C. Srivatsava, S. Saha and A. K. Jain, Prentice-hall, India.
- 5. Puri, Sharma, Pathania, Advance Physical chemistry
- 6. Advance Physical Chemistry, Gurdeep Raj, Pragati Pakashan, Meerut.

Paper-II (Analytical Chemistry)[CY-514]

- 1. Errors in Chemical Analysis and Statistical Evaluation of Data: Systematic and random errors, Accuracy and precision, Ways of expressing accuracy and precision, Normal error curve and its equation, Propagation of error, Useful statistical test: test of significance, the F test, the student 't' test, the chi-test, the correlation coefficient, confidence limit of the mean, comparison of two standard values, comparison of standard deviation with average deviation, comparison of mean with true values, significant figures.
- **2. Polarography:** Origin of polarography, Current-voltage relationship, Theory of polarographic waves (DC and sampled DC (test) polarograms), Instrumentation, Ilkovič equation, Qualitative and quantitative applications. Cyclic Voltammetry: Cell design, instrumentation, current-potential relation for linear sweep voltammetry (LSV), cyclic voltammetry, interpretation of voltammograms.
- **3. Separation Methods:** Principle of chromatography, Classifications of chromatography, Techniques of planar and column chromatography, Gas chromatography, Highperformance liquid chromatography.
- **4. Thermal Analysis:** Theory, methodology and applications of thermogravimetric analysis (TGA), Differential Thermal Analysis (DTA), and Differential scanning calorimetry (DSC). Principles, techniques and applications of thermometric titration methods.

- 1. Basic Concept of analytical Chemistry, S.M. Khopkar. Wiley Eastern Ltd.
- 2. H.H. Willard, L.L. Mirrit, J.A. Dean, Instrumental Methods of analysis, (CBS) publ.
- 3. Skoog and West, Principles of Instrumental Analysis, Saunders College Publishing, Philadelphia, London.
- 4. J.O'M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Plenum Press, New York.
- 5. H. Kaur, Instrumentation methods of chemical analysis, Pragati prakashan.

Paper-III (Inorganic Chemistry-II) [CY-516]

- 1. Co-ordination Chemistry: Double salts co-ordination compounds, Werner's theory of coordination compounds, IUPAC nomenclature, Effective atomic number (EAN), Isomerism in coordination compounds Valence bond theory and its limitations, crystal field theory, crystal field splitting of d-orbitals in octhahedral, tetrahedral and squre planar complexes, calculation of stabilizations energies (CFSE) for d¹ to d9 weak and strong fields, octhahedral complexes, spectrochemical series, Electronic spectra of 3d transition metal complexes, types of electronic transitions selection rules for electronic transition spectroscopic ground states for d¹ to d9 systems. Magnetism; Dia-, Para-, Ferro-, and anti ferromagnetism, quenching of orbital angular moment, spin orbital coupling, inorganic reactions mechanism; substitution reactions, trans effect and electron transfer reactions.
- **2. Nuclear Chemistry:** Nuclear reactions, Mass defect and Binding energy, Nuclear fission and fusion, Nuclear reactions, Radioisotopes and their applications.
- 3. Metal-Ligand bonding: Limitation of crystal field theory, Molecular orbital theory, Octahedral, tetrahedral and square planar complexes, π -bonding and molecular orbital theory.
- **4. Organometallic Chemistry:** Organoberyllium and silicon compounds: preparation stability and important reaction of transition metal alkyl and aryls. Metal carbonyls reactions, structure and bonding, vibrational spectra of metal carbonyls for structural elucidation.

- 1. Inorganic chemistry: Cotton & Wilikinson
- 2. Advanced inorganic chemistry: J. D. Lee
- 3. Selected topics in Inorganic chemistry: W. U. Malik, G. D. Tuli and R. D. Madan.
- 4. Advanced inorganic chemistry vol I& II: Gurdeep Raj
- 5. Advanced inorganic chemistry: Cotton & Wilikinson, Wiley

Paper-IV(Bio-inorganic Chemistry)[CY-518]

1. Bio-inorganic chemistry:

- I. **Metal Ions in Biological Systems:** (a) Essential and trace metals. (b) Na+/K+ Pump. (c) Heme proteins and oxygen uptake, structure and function of hemoglobin, , homocyanins and hemerythrin, model synthetic complexes of iron, cobalt and copper
- II. **Electron Transfer in Biology:** Structure and function of metalloproteins in electron transport processes-cytochromes and ion- sulphur proteins, synthetic models.
- III. **Nitrogenase:** Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.
- 2. Chemistry of less familiar metals: Chemistry of less familiar metals: Os, Ir, Ru, Rh, Pd,

3. Selected Topics

- I General method of preparation and important reactions (insertion reactions metathetical reactions, Lewis acid-base reactions, reactions with protic compounds) of metal and metalloid amides.
- II Preparation of important radio isotopes (1H³, 6C¹⁴, 11Na²², 15P³², 16S³⁵) and applications of coordination compounds of Tc⁹⁹ as imaging agents in Nuclear Medicine.

- 1. Inorganic chemistry: Cotton & Wilikinson
- 2. Advanced inorganic chemistry: J. D. Lee
- 3. Selected topics in Inorganic chemistry: W. U. Malik, G. D. Tuli and R. D. Madan.
- 4. Advanced inorganic chemistry vol I& II: Gurdeep Raj
- 5. Advanced inorganic chemistry: Cotton & Wilkinson, Wiley
- 6. Environmental chemistry and pollution control: S.S. Dara.
- 7. Environmental chemistry: C. Baird, W.H. Freeman & Co. Newyork
- 8. Environmental chemistry: B.K. Sharma & H. Kaur, Goel Publishing House Quantitative Inorganic Analysis, A.I. Vogel.
- 9 Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
- 10 10. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard & J.S.Valentine, University Science Books

- 1. Aromatic Electrophilic substitution: The arenium ion mechanism, Orientation and reactivity, energy profile diagram. The ortho / para ratio, ipso attack, orientation in other ring system, quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeir reaction, Gatterman-Koch reaction.
- **2. Aromatic Nucleophilic substitution:** Aromatic nucleophilic substitution, rearrangements involving nucleophilic aromatic substitution, Bombarger rearrangements, Bucherer reaction, Smiles rearrangements and Sommlett Hauser rearrangements.
- **3. Free Radical Reactions:** Alicyclic halogenation (NBS), oxidation of aldehyde to carboxylic acid, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salt. Sandemeyer reaction. Free radical rearrangement. Hunsdiecker reaction.
- **4. Addition to Carbon Carbon multiple bonds:** Mechanistic and stereochemical aspects of addition reaction involving electrophiles, Nucleophiles and free radicals, ragio-and chemoselectivity, orientation and reactivity, Addition to cyclopropane ring, Hydrogenation of double and triple bonds, Hydrogenation of aromatic ring, Hydroboration, Michael reaction, Sharpless asymmetric epoxidation
- **5. Named reactions:** Arndt-Eistert Synthesis, Bayer Villiger reaction, Favoraskii rearrangement, Claisen rearrangement, Baylis-Hillmann reaction, Mitsunobu reaction

- 1. Reactions and reagent in organic synthesis: O.P.Agarwal Goel Publishing House.
- 2. Stereochemistry of carbon compounds: Eliel, TMH Publishing Co. Ltd.
- 3. Synthetic organic chemistry: O.P.Agarwal Goel Publishing.
- 4. Mechanism in organic chemistry:Peter Syke
- 5. Advanced organic chemistry: Jerry March, Wiley
- 6. Synthetic reactions: House.

- 1. Carbohydrates: General reactions of Monosaccharides, epimerization, action of alkali, interconversion including Kiliani synthesis, Wohl's ,Ruff's method, ring structre of aldose, determination of the size of ring by methylation method and periodate oxidation method, mutarotation, structure establishment of Diasaccharides: Sucrose, Maltose, Lactose, and Polysaccharides: Starch and cellulose
- 2. Heterocyclic compounds: Introduction, nomenclature, Synthesis, reactions and structure of Heterocyclics having one heteroatom e.g. Pyrole, furan, Quinoline, Indoles; synthesis and reaction of hetrocyclic containing two different hetro atom viz. Thiazole group: examples Thiazole, thiazolines, thiazolidines, benzothiazoles and isothiazoles; hetrocyclics containing three hetro atoms Triazole group: Triazole, benzotriazole and oxadiazole
- **Proteins:** Amino acids, classification of amino acids, Synthesis of amino acids, properties of amino acids, Classification of Proteins, peptide linkage, primary structure of peptides, Synthesis of Peptides, Oxytocin, Insulin

4. Biocatalysts in Green Chemistry:

Advantages, Nomenclature, classification, efficiency, specificity-stereospecificity and reaction specificity, substrate specificity, mechanics of enzyme action, coenzymes with structure elucidation of coenzyme I or Co-Zymase DPN, Biochemical oxidations, Biochemical reductions.

- 1. Organic Chemistry: R.T. Morrison and R.N. Boyd P.H. Ltd.
- 2. Topics in Organic Chemistry: Fieser and Fieser, Reinhold.
- 3. Organic Chemistry: Vol. I & II: I.L.Finar, Elbs with Longmann Pub.