SEMESTER V&VI

B. SC. PHYSICAL SCIENCES

(CHEMISTRY)

Semester V

CCL-503(i)
Discipline Specific Course-I(i)
POLYMER CHEMISTRY-I
Credits: 02; 30 Hrs (2Hrs /week)

Marks for Major Test (External): 80
Marks for Internal Exam: 20
Time: 3Hrs

Note: ***The examiner is requested to set nine questions in all, selecting two questions from each UNIT and one compulsory question (Question No.1 based on entire syllabus will consist of eight short answer type questions each of two marks). The candidate is required to attempt five questions in all selecting one from each UNIT and the compulsory Question No.1.***

UNIT-I

Introduction and history of polymeric materials:
Different schemes of classification of polymers, Polymer nomenclature, Molecular forces and chemical bonding in polymers, Texture of polymers.
Nature and structure of polymers-Structure Property relationships.

(7 Hours)

UNIT-II

Functionality and its importance:
Criteria for synthetic polymer formation, classification of polymerization processes, Relationships between functionality, extent of reaction and degree of polymerization.Bi-functional systems, Poly-functional systems.
Properties of Polymers (Physical, thermal, flow & mechanical properties).

(8 Hours)

UNIT-III

Brief introduction to preparation, structure, properties and application of the following polymers: polyolefins, polystyrene and styrene copolymers, poly(vinyl chloride) and related polymers, poly(vinyl acetate) and related polymers, acrylic polymers, fluoro polymers, polyamides and related polymers.

(8 Hours)

UNIT-IV

Polycarbonates,Phenol formaldehyde resins (Bakelite, Novalac), polyurethanes, silicone polymers, polydienes, Conducting Polymers, [polyacetylene, polyaniline, poly(p-phenylene sulphide polypyrrole, polythiophene)].

(7 Hours)

Reference Books:

- Seymour, R.B.&Carraher, C.E. *Polymer Chemistry: An Introduction,* Marcel Dekker, Inc. New York, 1981.
- Odian, G. *Principles of Polymerization*, 4th Ed. Wiley, 2004.
- Billmeyer, F.W. *Textbook of Polymer Science*, 2nd Ed. Wiley Interscience, 1971.
- Ghosh, P. *Polymer Science & Technology*, Tata McGraw-Hill Education, 1991.
- Lenz, R.W. *Organic Chemistry of Synthetic High Polymers.* Interscience Publishers, New York, 1967.

CCL-504(i)
Discipline Specific Course-I(i)
POLYMER CHEMISTRY-II
Credits: 02; 30 Hrs (2Hrs /week)

Marks for Major Test (External): 80
Marks for Internal Exam: 20
Time: 3Hrs

Note: The examiner is requested to set nine questions in all, selecting two questions from each UNIT and one compulsory question (Question No.1 based on entire syllabus will consist of eight short answer type questions each of two marks). The candidate is required to attempt five questions in all selecting one from each UNIT and the compulsory Question No.1.

UNIT-I

Kinetics of Polymerization: Mechanism and kinetics of step growth, radical chain growth, ionic chain (both cationic and anionic) and coordination polymerizations, Mechanism and kinetics of copolymerization, polymerization techniques.

(8 Hours)

UNIT-II

Crystallization and crystallinity: Determination of crystalline melting point and degree of crystallinity, Morphology of crystalline polymers, Factors affecting crystalline melting point.
Glass transition temperature (Tg) and determination of Tg, Free volume theory, WLF equation, Factors affecting glass transition temperature (Tg).

(7 Hours)

UNIT-III

Determination of molecular weight of polymers (M_n, M_w, etc) by end group analysis, viscometry, light scattering and osmotic pressure methods.Molecular weight distribution and its significance.Polydispersity index.

(7 Hours)

UNIT-IV

Polymer Solution: Criteria for polymer solubility, Solubility parameter, Thermodynamics of polymer solutions, entropy, enthalpy, and free energy change of mixing of polymers solutions, Flory- Huggins theory, Lower and Upper critical solution temperatures.

(8 Hours)

Reference Books:

- Seymour, R.B.&Carraher, C.E. *Polymer Chemistry: An Introduction,* Marcel Dekker, Inc. New York, 1981.
- Odian, G. *Principles of Polymerization*, 4th Ed. Wiley, 2004.
- Billmeyer, F.W. *Textbook of Polymer Science*, 2nd Ed. Wiley Interscience, 1971.
- Ghosh, P. *Polymer Science & Technology*, Tata McGraw-Hill Education, 1991.
- Lenz, R.W. *Organic Chemistry of Synthetic High Polymers.* Interscience Publishers, New York, 1967.

CCP-509(i)
PRACTICAL-V(i)
CHEMISTRY DSC LAB V(i)
POLYMER CHEMISTRY
Credits: 02; 60Hrs (4 Hrs /week)

Marks (External): 100
Time: 6Hrs

I. Polymer synthesis

1. Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA) / Methyl Acrylate (MA) / Acrylic acid (AA).
   a. Purification of monomer
   b. Polymerization using benzoyl peroxide (BPO) / 2,2'-azo-bisisobutylonitrile (AIBN)
2. Preparation of nylon 66/6
3. Interfacial polymerization, preparation of polyester from isophthaloyl chloride (IPC) and phenolphthalein
   a. Preparation of IPC
   b. Purification of IPC
   c. Interfacial polymerization
4. Redox polymerization of acrylamide
5. Precipitation polymerization of acrylonitrile
6. Preparation of urea-formaldehyde resin
7. Preparation of novalac resin/resold resin
8. Microscale emulsion polymerization of poly(methylacrylate).

II. Polymer characterization

1. Determination of molecular weight by viscometry:
   a. Polyacrylamide-aq. $NaNO_2$ solution
   b. (Poly vinyl proplylidine (PVP) in water
2. Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of "head-to-head" monomer linkages in the polymer.
3. Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).

III. Polymer analysis

1. Estimation of the amount of HCHO in the given solution by sodium sulphite method
2. Instrumental Techniques
3. Preparation of polyacrylamide and its electrophoresis

*at least 7 experiments to be carried out.

Reference Books:

- M.P. Stevens, *Polymer Chemistry: An Introduction*, 3rd Ed., Oxford University Press, 1999.
- H.R. Allcock, F.W. Lampe & J.E. Mark, *Contemporary Polymer Chemistry*, 3rd ed. Prentice-Hall (2003)
- F.W. Billmeyer, *Textbook of Polymer Science*, 3rded.Wiley-Interscience (1984)
- J.R. Fried, *Polymer Science and Technology*, 2nded.Prentice-Hall (2003)
- P. Munk& T.M. Aminabhavi, *Introduction to Macromolecular Science*, 2nded.John Wiley & Sons (2002)
- L. H. Sperling, *Introduction to Physical Polymer Science*, 4thed.John Wiley & Sons (2005)
- M.P. Stevens, *Polymer Chemistry: An Introduction*3rded.Oxford University Press (2005).
- Seymour**/** Carraher's Polymer Chemistry, 9th ed.by Charles E. Carraher, Jr. (2013).

CCL-503(ii)
Discipline Specific Course-I(ii)
Chemistry of Main Group Elements, Theories of Acids and Bases-I
Credits: 02; 30 Hrs (2Hrs /week)

Marks for Major Test (External): 80
Marks for Internal Exam: 20
Time: 3Hrs

Note: ***The examiner is requested to set nine questions in all, selecting two questions from each UNIT and one compulsory question (Question No.1 based on entire syllabus will consist of eight short answer type questions each of two marks). The candidate is required to attempt five questions in all selecting one from each UNIT and the compulsory Question No.1.***

UNIT-I

Acids and Bases: Bronsted–Lowry concept, conjugate acids and bases, relative strengths of acids and bases, effects of substituent and solvent, differentiating and levelling solvents. Lewis acid-base concept, classification of Lewis acids and bases, Lux-Flood concept and solvent system concept.Hard and soft acids and bases (HSAB concept), applications of HSAB process.

(7 Hours)

UNIT-II

General Principles of Metallurgy: Chief modes of occurrence of metals based on standard electrode potentials, Ellingham diagrams for reduction of metal oxides using carbon and carbon monoxide as reducing agents.
Hydrometallurgy with reference to cyanide process for gold and silver. Methods of purification of metals (Al, Pb, Ti, Fe, Cu, Ni, Zn, Au): electrolytic refining, zone refining, van Arkel-de Boer process, Parting Process, Mond's process and Kroll Process.

(8 Hours)

UNIT-III

***s*- and *p*-Block Elements**
Periodicity in *s*- and *p*-block elements with respect to electronic configuration, atomic and ionic size, ionization enthalpy, electron gain enthalpy, electronegativity (Pauling scale).
General characteristics of *s*-block metals like density, melting and boiling points, flame colour and reducing nature.
Oxidation states of *s*- and *p*-block elements, inert-pair effect, diagonal relationships and anomalous behaviour of first member of each group. Allotropy in C, P and S.

(7 Hours)

UNIT-IV

Complex forming tendency of *s* block elements and a preliminary idea of crown ethers and cryptates, structures of basic beryllium acetate, salicylaldehyde/ acetylacetonato complexes of Group 1 metals.
Solutions of alkali metals in liquid ammonia and their properties.
Common features, such as ease of formation, solubility and stability of oxides, peroxides, superoxides, sulphates and carbonates of *s*-block metals.

(8 Hours)

Recommended texts:

- Lee, J.D. *Concise Inorganic Chemistry* ELBS, 1991.
- Cotton, F.A., Wilkinson, G. &Gaus, P.L. *Basic Inorganic Chemistry*, 3rd ed., Wiley.
- Douglas, B.E., McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry*, John Wiley & Sons.
- Greenwood, N.N. &Earnshaw. *Chemistry of the Elements*, ButterworthHeinemann. 1997.
- Rodger, G.E. *Inorganic and Solid State Chemistry*, Cengage Learning India Edition, 2002.
- Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry* 4thEd.,Pearson, 2010.

Atkin, P. *Shriver & Atkins' Inorganic Chemistry* 5th Ed. Oxford University Press (2010).

CCL-504(ii)
Discipline Specific Course-II(ii)
Chemistry of Main Group Elements-II
Credits: 02; 30 Hrs (2Hrs /week)

Marks for Major Test (External): 80
Marks for Internal Exam: 20
Time: 3Hrs

Note: *The examiner is requested to set nine questions in all, selecting two questions from each UNIT and one compulsory question (Question No.1 based on entire syllabus will consist of eight short answer type questions each of two marks). The candidate is required to attempt five questions in all selecting one from each UNIT and the compulsory Question No.1.*

UNIT-I

Structure, bonding and properties (acidic/ basic nature, oxidizing/ reducing nature and hydrolysis of the following compounds and their applications in industrial and environmental chemistry wherever applicable:
Diborane and concept of multicentre bonding, hydrides of Groups 13 (EH_3), 14, 15, 16 and 17.
Oxides of N and P, Oxoacids of P, S and Cl.

(8 Hours)

UNIT-II

Halides and oxohalides of P and S (PCl_3, PCl_5, $SOCl_2$ and SO_2Cl_2) Interhalogen compounds.
A brief idea of pseudohalides

(7 Hours)

UNIT-III

Noble gases: Rationalization of inertness of noble gases, clathrates, preparation and properties of XeF_2, XeF_4 and XeF_6 ,bonding in these compounds using VBT and shapes of noble gas compounds using VSEPR Theory

(7 Hours)

UNIT-IV

Inorganic Polymers: Types of inorganic polymers and comparison with organic polymers, structural features, classification and important applications of silicates. Synthesis, structural features and applications of silicones.Borazines and cyclophosphazenes – preparation, properties and reactions. Bonding in $(NPCl_2)_3$.

(8 Hours)

Recommended texts:

- Lee, J.D. *Concise Inorganic Chemistry* ELBS, 1991.
- Cotton, F.A., Wilkinson, G. &Gaus, P.L. *Basic Inorganic Chemistry*, 3rd ed., Wiley.
- Douglas, B.E., McDaniel, D.H. & Alexander, J.J. *Concepts and Models in Inorganic Chemistry*, John Wiley & Sons.
- Greenwood, N.N. &Earnshaw. *Chemistry of the Elements*, ButterworthHeinemann. 1997.
- Rodger, G.E. *Inorganic and Solid State Chemistry*, Cengage Learning India Edition, 2002.
- Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry* 4thEd.,Pearson, 2010.
- Atkin, P. *Shriver & Atkins' Inorganic Chemistry* 5th Ed. Oxford University Press (2010).

CCP-509(ii)
PRACTICAL-V(ii)
CHEMISTRY DSC LAB V
Chemistry of Main Group Elements, Theories of Acids and Bases
Credits: 02; 60 Hrs (4 Hrs /week)

Marks (External): 100
Time: 6Hrs

1. Iodometric estimation of potassium dichromate and copper sulphate
2. Iodimetric estimation of antimony in tartaremetic
3. Estimation of amount of available chlorine in bleaching powder and household bleaches
4. Estimation of iodine in iodized salts.
5. Iodimetric estimation of ascorbic acid in fruit juices.
6. Estimation of dissolved oxygen in water samples.
7. Gravimetric estimation of sulphate as barium sulphate.
8. Gravimetric estimation of aluminium as oximato complex
9. Preparation of the following: potash alum, chrome alum, tetraamminecopper(II) sulphate monohydrate, potassium trioxalatoferrate(III) (any two, including one double salt and one complex).

Recommended Texts:

- Svehla, G. *Vogel's Qualitative Inorganic Analysis*, Pearson Education, 2012.
- Mendham, J. *Vogel's Quantitative Chemical Analysis*, Pearson, 2009.

CCS-505(i)
Skill Enhancement Course-I
PESTICIDE CHEMISTRY (Theory)
Credits: 02; 30 Hrs (2Hrs /week)

Total Marks: 100

Marks (External): 50

Examination Time: 2Hrs

Note: The examiner is requested to set five questions in all, selecting two questions from each UNIT and one compulsory question (Question No.1 based on entire syllabus will consist of ten short answer type questions each of two marks). The candidate is required to attempt three questions in all selecting one from each UNIT and the compulsory Question No.1.

UNIT-I

General introduction to pesticides (natural and synthetic), benefits and adverse effects, changing concepts of pesticides.

UNIT-II

Structure activity relationship, synthesis and uses of representative pesticides in the following classes: Organochlorines (DDT, Gammexene, Aldrin, Dialdrin); Organophosphates (Malathion, Parathion); Carbamates (Carbofuran and carbaryl); Quinones (Chloranil), Anilides (Alachlor and Butachlor).

Marks (Internal): 50

Skill Enhancement Course-I
PESTICIDE CHEMISTRY (Practicals)

1. To calculate acidity/alkalinity in given sample of pesticide formulations as per BIS specifications.
2. Preparation of simple organophosphates, phosphonates and thiophosphates

Reference Book

- Cremlyn, R. *Pesticides. Preparation and Modes of Action*, John Wiley & Sons, New York, 1978.

CCS-505(ii)
Skill Enhancement Course-III
FUEL CHEMISTRY (Theory)
Credits: 02; 30 Hrs (2Hrs /week)

Total Marks: 100

Marks (External): 50

Time: 2 Hrs

Note: The examiner is requested to set five questions in all, selecting two questions from each UNIT and one compulsory question (Question No.1 based on entire syllabus will consist of ten short answer type questions each of two marks). The candidate is required to attempt three questions in all selecting one from each UNIT and the compulsory Question No.1.

UNIT-I

Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value.

Coal: Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal. Coal gas, producer gas and water gas—composition and uses. Fractionation of coal tar, uses of coal tar bases chemicals, requisites of a good metallurgical coke, Coal gasification (Hydro gasification and Catalytic gasification), Coal liquefaction and Solvent Refining.

Petroleum and Petrochemical Industry: Composition of crude petroleum, Refining and different types of petroleum products and their applications.

UNIT-II

Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking), Reforming Petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels. Petrochemicals: Vinyl acetate, Propylene oxide, Isoprene, Butadiene, Toluene and its derivatives Xylene.

Lubricants: Classification of lubricants, lubricating oils (conducting and nonconducting) Solid and semisolid lubricants, synthetic lubricants.
Properties of lubricants (viscosity index, cloud point, pore point) and their determination.

Marks (Internal): 50

Skill Enhancement Course-III
FUEL CHEMISTRY (Practicals)

Properties of lubricants (viscosity index, cloud point, pore point) and their determination.

Reference Books:

- Stocchi, E. *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK (1990).
- Jain, P.C. & Jain, M. *Engineering Chemistry*DhanpatRai& Sons, Delhi.
- Sharma, B.K. & Gaur, H. *Industrial Chemistry,* Goel Publishing House, Meerut (1996).

Semester VI
CCL-603(i)
Discipline Specific Course-III(i)
ORGANOMETALLICS AND BIOINORGANIC CHEMISTRY
Credits: 02; 30 Hrs (2Hrs /week)

Marks for Major Test (External): 80
Marks for Internal Exam: 20
Time: 3Hrs

Note: The examiner is requested to set nine questions in all, selecting two questions from each UNIT and one compulsory question (Question No.1 based on entire syllabus will consist of eight short answer type questions each of two marks). The candidate is required to attempt five questions in all selecting one from each UNIT and the compulsory Question No.1.

UNIT-I

Chemistry of 3d metals

Oxidation states displayed by Cr, Fe, Co, Ni and Co.
A study of the following compounds (including preparation and important properties);
Peroxo compounds of Cr, $K_2Cr_2O_7$, $KMnO_4$, $K_4[Fe(CN)_6]$, sodium nitroprusside, $[Co(NH_3)_6]Cl_3$, $Na_3[Co(NO_2)_6]$.

(8 Hours)

UNIT-II

Organometallic Compounds

Definition and Classification with appropriate examples based on nature of metalcarbon bond (ionic, s, p and multicentre bonds). Structures of methyl lithium, Zeiss salt and ferrocene. EAN rule as applied to carbonyls.

(7 Hours)

UNIT-III

Preparation, structure, bonding and properties of mononuclear and polynuclear carbonyls of 3d metals.p-acceptor behaviour of carbon monoxide. Synergic effects (VB approach)-(MO diagram of CO can be referred to for synergic effect to IR frequencies).

(7 Hours)

UNIT-IV

Bio-Inorganic Chemistry

A brief introduction to bio-inorganic chemistry. Role of metal ions present in biological systems with special reference to Na^+, K^+ and Mg^{2+} ions: Na/K pump; Role of Mg^{2+} ions in energy production and chlorophyll. Role of Ca^{2+} in blood clotting, stabilization of protein structures and structural role (bones).

(8 Hours)

Reference Books:

- James E. Huheey, Ellen Keiter& Richard Keiter: *Inorganic Chemistry: Principles of Structure and Reactivity,* Pearson Publication.
- G.L. Miessler& Donald A. Tarr: *Inorganic Chemistry,* Pearson Publication.
- J.D. Lee: *A New Concise Inorganic Chemistry,* E.L.B.S.
- F.A. Cotton & G. Wilkinson: *Basic Inorganic Chemistry*, John Wiley & Sons.

CCL-604(i)
Discipline Specific Course-IV(i)
POLYNUCLEAR HYDROCARBONS AND UV, IR SPECTROSCOPY
Credits: 02; 30 Hrs (2Hrs /week)

Marks for Major Test (External): 80
Marks for Internal Exam: 20
Time: 3Hrs

Note: The examiner is requested to set nine questions in all, selecting two questions from each UNIT and one compulsory question (Question No.1 based on entire syllabus will consist of eight short answer type questions each of two marks). The candidate is required to attempt five questions in all selecting one from each UNIT and the compulsory Question No.1.

UNIT-I

Polynuclear and heteronuclear aromatic compounds:
Properties of the following compounds with reference to electrophilic and nucleophilic substitution: Naphthalene, Anthracene, Furan, Pyrrole, Thiophene, and Pyridine.

(8 Hours)

UNIT-II

Active methylene compounds:
Preparation: Claisen ester condensation. Keto-enoltautomerism.
Reactions: Synthetic uses of ethyl acetoacetate (preparation of non-hetero molecules having upto 6 carbon).

(7 Hours)

UNIT-III

Application of Spectroscopy to Simple Organic Molecules
Application of visible, ultraviolet and infrared spectroscopy in organic molecules. Electromagnetic radiations, electronic transitions, λ_{max}&ε_{max}, chromophore, auxochrome, bathochromic and hypsochromic shifts. Application of electronic spectroscopy and Woodward rules for calculating λ_{max} of conjugated dienes and α,β-unsaturated compounds.

(7 Hours)

UNIT-IV

Infrared radiation and types of molecular vibrations, functional group and fingerprint region. IR spectra of alkanes, alkenes and simple alcohols (inter and intramolecular hydrogen bonding), aldehydes, ketones, carboxylic acids and their derivatives (effect of substitution on >C=O stretching absorptions).

(8 Hours)

Reference Books:

- I.L. Finar: *Organic Chemistry* (Vol. I & II), E.L.B.S.
- John R. Dyer: *Applications of Absorption Spectroscopy of Organic Compounds,* Prentice Hall.
- R.M. Silverstein, G.C. Bassler& T.C. Morrill*: Spectroscopic Identification of Organic Compounds*, John Wiley & Sons.
- R.T. Morrison & R.N. Boyd: *Organic Chemistry,* Prentice Hall.
- Peter Sykes: *A Guide Book to Mechanism* in *Organic Chemistry,* Orient Longman.
- ArunBahl and B. S. Bahl: *Advanced Organic Chemistry,* S. Chand.

CCP-609(i)
PRACTICAL-VI(i)
CHEMISTRY DSC LAB VI
Organometallics, Bioinorganic Chemistry, Polynuclear Hydrocarbons and UV, IR Spectroscopy
Credits: 02; 60 Hrs (4Hrs /week)

Marks (External): 100
Time: 6Hrs

Section A: Inorganic Chemistry

1. Separation of mixtures by chromatography: Measure the R_f value in each case. (Combination of two ions to be given)
a. Paper chromatographic separation of Fe^{3+}, $A1^{3+}$ and Cr^{3+} or
b. Paper chromatographic separation of Ni^{2+}, Co^{2+}, Mn^{2+} and Zn^{2+}
2. Preparation of any two of the following complexes and measurement of their conductivity:
a. tetraamminecarbonatocobalt (III) nitrate
b. tetraamminecopper (II) sulphate
c. potassium trioxalatoferrate (III) trihydrate

Compare the conductance of the complexes with that of M/1000 solution of NaCl, $MgCl_2$ and $LiCl_3$.

Section B: Organic Chemistry

Systematic Qualitative Organic Analysis of Organic Compounds possessing monofunctional groups (-COOH, phenolic, aldehydic, ketonic, amide, nitro, amines) and preparation of one derivative.

Reference Books:

- A.I. Vogel: Qualitative Inorganic Analysis, Prentice Hall, 7th Edn.
- A.I. Vogel: Quantitative Chemical Analysis, Prentice Hall, 6th Edn.
- Vogel, A.I., Tatchell, A.R., Furnis, B.S., Hannaford, A.J. & Smith, P.W.G., *Textbook of Practical Organic Chemistry*, Prentice-Hall, 5th edition, 1996.
- Mann, F.G. & Saunders, B.C. *Practical Organic Chemistry* Orient-Longman, 1960.

CCL-603(ii)
Discipline Specific Course-III(ii)
QUANTUM CHEMISTRY
Credits: 02; 30 Hrs (2Hrs /week)

Marks for Major Test (External): 80
Marks for Internal Exam: 20
Time: 3Hrs

Note: The examiner is requested to set nine questions in all, selecting two questions from each UNIT and one compulsory question (Question No.1 based on entire syllabus will consist of eight short answer type questions each of two marks). The candidate is required to attempt five questions in all selecting one from each UNIT and the compulsory Question No.1.

UNIT-I

Postulates of quantum mechanics, quantum mechanical operators, Schrödinger equation and its application to free particle and "particle-in-a-box" (rigorous treatment), quantization of energy levels, zero-point energy and Heisenberg Uncertainty principle; wavefunctions, probability distribution functions, nodal properties, Extension to two and three dimensional boxes, separation of variables, degeneracy.

(8 Hours)

UNIT-II

Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wave functions. Vibrational energy of diatomic molecules and zero-point energy.
Angular momentum: Commutation rules, quantization of square of total angular momentum and z-component.
Rigid rotator model of rotation of diatomic molecule.Schrödinger equation.

(7 Hours)

UNIT-III

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part, quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus.
Setting up of Schrödinger equation for many-electron atoms (He, Li). Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).

(7 Hours)

UNIT-IV

Chemical bonding: Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of H_2^+. Bonding and antibonding orbitals.Qualitative extension to H_2. Comparison of LCAO-MO and VB treatments of H_2 (only wavefunctions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB).Qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules (HF, LiH).

(8 Hours)

Reference Books:

- Chandra, A. K. *Introductory Quantum Chemistry* Tata McGraw-Hill (2001).
- House, J. E. *Fundamentals of Quantum Chemistry* 2nd Ed. Elsevier: USA (2004).
- Lowe, J. P. & Peterson, K. *Quantum Chemistry*, Academic Press (2005).

CCL-604(ii)
Discipline Specific Course-IV(ii)
SPECTROSCOPY & PHOTOCHEMISTRY
Credits: 02; 30 Hrs (2Hrs /week)

Marks for Major Test (External): 80
Marks for Internal Exam: 20
Time: 3Hrs

Note: The examiner is requested to set nine questions in all, selecting two questions from each UNIT and one compulsory question (Question No.1 based on entire syllabus will consist of eight short answer type questions each of two marks). The candidate is required to attempt five questions in all selecting one from each UNIT and the compulsory Question No.1.

UNIT-I

Molecular Spectroscopy:

Interaction of electromagnetic radiation with molecules and various types of spectra; Born-Oppenheimer approximation.

Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.

Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

(8 Hours)

UNIT-II

Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.

Electronic spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model.

(7 Hours)

UNIT-III

Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Larmor precession, chemical shift and low resolution spectra, different scales, spinspin coupling and high resolution spectra, interpretation of PMR spectra of organic molecules.

Electron Spin Resonance (ESR) spectroscopy: Its principle, hyperfine structure, ESR of simple radicals.

(8 Hours)

UNIT-IV

Photochemistry

Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws, of photochemistry, quantum yield, actinometry, examples of low and high quantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitised reactions, quenching. Role of photochemical reactions in biochemical processes, photostationary states, chemiluminescence.

(7 Hours)

Reference Books:

- Banwell, C. N. &McCash, E. M. *Fundamentals of Molecular Spectroscopy* 4th Ed. Tata McGraw-Hill: New Delhi (2006).
- Kakkar, R. *Atomic & Molecular Spectroscopy*: *Concepts & Applications*, Cambridge University Press (2015).

CCP-609(ii)
Practical-VI(ii)
CHEMISTRY DSE LAB 6B: QUANTUM CHEMISTRY, SPECTROSCOPY & PHOTOCHEMISTRY
Credits: 02; 60 Hrs (4Hrs /week)

Marks (External): 100
Time: 6Hrs

UV/Visible spectroscopy

1. Study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) and determine the λ_{max} values. Calculate the energies of the two transitions in different units (J molecule^{-1}, kJ mol^{-1}, cm^{-1}, eV).
2. Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$.
3. Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.

Colorimetry

1. Verify Lambert-Beer's law and determine the concentration of $CuSO_4$ / $KMnO_4$ / $K_2Cr_2O_7$ in a solution of unknown concentration
2. Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture.
3. Study the kinetics of iodination of propanone in acidic medium.
4. Determine the amount of iron present in a sample using 1,10-phenathroline.
5. Determine the dissociation constant of an indicator (phenolphthalein).
6. Analyse the given vibration-rotation spectrum of HCl(g)

Reference Books

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- Khosla, B. D.; Garg, V. C. &Gulati, A., *Senior Practical Physical Chemistry,* R. Chand & Co.: New Delhi (2011).
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