GAYATRI VIDYA PARISHAD COLLEGE FOR DEGREE AND PG COURSES (A) M.Sc. ORGANIC OF CHEMISTRY SYLLABUS I- SEMESTER PAPER - I: GENERAL CHEMISTRY – I QUANTUM CHEMISTRY (Effective from 2020-21 admitted batch)

(Effective from 2020-21 admitted batch)		
Credits : 4		Theory : 4 Hours
Max Marks : 100	External : 80	Internal : 20

Course Objectives:

- 1. To know the concepts of classical and quantum mechanics
- 2. To solve the simple quantum mechanical problems such as simple harmonic oscillator, particle in a 1D-box, rigid rotor, H atom etc.
- 3. To calculate energy and wave functions of multi electron systems using perturbation and variation theorems.

UNIT-I

Wave equation – interpretation of wave function – properties of wave function – normalization and orthogonalisation - operators –linear and non linear - commutators of operators. Postulates of quantum mechanics - setting up of operators - observables – Hermitian operator – Eigen values of Hermitian operator.

UNIT-II

Wave mechanics of simple systems with constant potential energy, particle in a one dimensional box - factors influencing color –transition. Dipole integral - symmetry arguments in deriving the selection rules – Concept of tunneling – particle in a three dimensional box - rigid rotor - wave mechanics of systems with variable potential energy - simple harmonic oscillator – solution of wave equation – selection rules.

UNIT-III

Hydrogen atom - solution of R(r), $\phi(\phi)$ and $\theta(\theta)$ equations – probability density in orbitals – shapes of orbitals. Perturbation theory – time independent perturbations (only first order perturbation is to be dealt with) – application to ground state energy of helium atom – variation principle – applications – calculation of zero point energy of harmonic oscillator – many electron atoms – Hartree-Fock self-consistent field method (qualitative treatment only)

UNIT-IV

Valence bond approach – directed valence – hybridization – covalent bond – calculation of ionic and covalent bond contribution in hydrogen molecule. Molecular orbital theory – LCAO approximation – hydrogen molecule ion – hydrogen molecule (basic concepts only), electronic transitions in the hydrogen molecule.

Course Outcomes:

- 1. The difference between classical and quantum mechanics and the connection to be made to quantum mechanical operators to observables
- 2. To solve the simple quantum mechanical problems such as simple harmonic oscillator, particle in a 1D-box, rigid rotor, H atom etc.

- 3. Calculation of energy and wave functions of multi electron systems using perturbation and variation theorems.
- 4. Connection between common approximation methods and standard chemical frameworks

- 1. Introductory Quantum Chemistry, A.K. Chandra, 4th Edition, Tata McGraw Hill, New Delhi (2006).
- 2. Quantum Chemistry and Spectroscopy, M.S. Pathania, Vishal Publishing Co., New Delhi (1981).
- 3. Quantum Chemistry, H. Eyring, J. Walter and G. Kimball, John Wiely & Sons, New York, (1944)
- 4. Fundamentals of Quantum Chemistry, R. Anantharaman, Macmillan Publishers India Ltd., New Delhi (2000)
- 5. Quantum Chemistry, Ira N. Levine, 7th Edition, Pearson, New Delhi, (2013)

GAYATRI VIDYA PARISHAD COLLEGE FOR DEGREE AND PG COURSES (A) M.Sc. ORGANIC OF CHEMISTRY SYLLABUS I- SEMESTER PAPER - II: INORGANIC CHEMISTRY – I (Effective from 2020-21 admitted batch)

Credits : 4		Theory : 4 Hours
Max Marks : 100	External: 80	Internal : 20

Course Objectives:

- 1. Importance of VSEPR, VBT and MO theory.
- 2. New concepts of inorganic chains, rings, cages and fundamentals of the chemistry of the main group elements.
- 3. To know the importance of CFT, and CFSE values.
- 4. Determination of spectral properties and magnetic properties of the complex compounds.

UNIT I

Term Symbols: Russell – Saunders coupling – derivation of term symbols for various configurations, and predicting spectroscopic ground states. Structure & Bonding: Application of VSEPR, Valance Bond and Molecular orbital theories in explaining the structure of simple molecules – role of 'p' and'd' orbitals in pi bonding.

UNIT II

Inorganic cage and ring compounds – preparation, structure and reactions of boranes, carboranes, metallocarboranes. Electron counting in boranes – Wades rules (Polyhedral skeletal electron pair theory). Boron – nitrogen ($H_3B_3N_3H_3$), Phosphorous – nitrogen ($N_3P_3Cl_6$) and sulphur – nitrogen (S_4N_4 , (SN)_x) cyclic compounds - Intercalation compounds.

UNIT III

Coordination compounds: Crystal field theory – crystal field splitting patterns in octahedral, tetrahedral, tetragonal, square planer, square pyramidal and trigonal bipyramidal geometries. Determination of crystal field stabilization energies. Factors affecting crystal field splitting energies – spectrochemical series – Jahn–Tellar effect, nephelauxetic effect – ligand field theory - Application of MO theory to octahedral complexes involving σ and π -bonding.

UNIT IV

Electronic spectra of transition metal complexes: selection rules, breakdown of selection rules - Orgel and Tanabe Sugano diagrams for $d^1 - d^9$ octahedral and tetrahedral transition metal complexes of 3d series – Calculation of Dq, B and β parameters. Charge transfer spectra. Magnetic properties of transition and inner transition metal complexes - spin and orbital moments - quenching of orbital momentum by crystal fields in complexes.

Course Outcomes:

Students will gain an understanding of

- 1. Predicting geometries of molecules using VSEPR, VBT and MO theory.
- 2. Learning various aspects of inorganic chains, rings, cages and fundamentals of the chemistry of the main group elements.
- 3. Splitting of d-orbitals in various geometries, and to predict the stability of complexes.
- 4. Determination of spectral properties of complex compounds and predict the colour, magnetic properties of the complex compounds.

- 1. Advanced Inorganic Chemistry, F.A. Cotton and R. G. Wilkinson, 4th Edition, John Wiley & Sons, New York (1980).
- 2. Inorganic Chemistry, J.E. Huheey. 3rd Edition, Harper International Edition, London (1983).
- 3. Theoretical Inorganic Chemistry, M.C. Day and J. Selbin, 2nd Edition, Affiliated East-West Press Pvt. Ltd., New Delhi.
- 4. Inorganic Chemistry, D.F. Shriver and P.W. Atkins, Oxford University Press, Oxford (1999).
- 5. Inorganic Chemistry, G.L. Miessler and D.A. Tarr, 3rd Edition, Pearson, New Delhi (2008).

GAYATRI VIDYA PARISHAD COLLEGE FOR DEGREE AND PG COURSES (A) M.Sc. ORGANIC OF CHEMISTRY SYLLABUS I- SEMESTER PAPER III: ORGANIC CHEMISTRY – I (Effective from 2020-21 admitted batch)

Credits : 4		Theory : 4 Hours
Max Marks : 100	External : 80	Internal : 20

Course Objectives:

- 1. To learn organic reactions reagents intermediates and aromatic compounds
- 2. To have a understanding how molecules are arranged using stereochemistry
- 3. To know the structure synthesis and reactivity of heterocyclic molecules
- 4. To know the synthesis, structure elucidation of natural products.

UNIT I

Structure and Reactivity: Introduction to types of organic reactions and reagents - reactive intermediates – generation and stability of carbocations, carbanions, free radicals, carbenes and nitrenes - concept of resonance - hyper conjugation - inductive and mesomeric effects - aromaticity - Huckel's rule for aromaticity in benzenoid and non-benzenoid compounds - anti aromaticity and homo-aromaticity.

UNIT II

Stereochemistry and stereoisomerism:

Molecular representations - Wedge, Fischer, Newman and Saw-horse formulae - their description and interconversions - conformational isomerism and analysis in acyclic and simple cyclic systems - ethane and substituted ethanes, cyclopentane, cyclohexane, cycloheptane, cyclooctane and decalins - optical isomerism - optical activity - molecular dissymmetry and chirality – elements of symmetry - D,L and R,S configurations – relative and absolute configurations - optical isomerism due to asymmetric carbon atoms - optical isomerism in biphenyl, allenes and spirans - optical isomerism of nitrogenous compounds - racemization and resolution - geometrical isomerism and E,Z configurations, properties of geometrical isomers.

UNIT III

Chemistry of heterocyclic compounds, synthesis and reactivity of pyridine, quinoline, indole, benzofuran, pyrazole, imidazole, oxazole, thiazole, pyrimidine, pyrazine,

UNIT IV

Chemistry of some typical natural products - study of the following compounds involving their isolation - structure elucidation - synthesis and biogenesis **Flavonoids:** Quercetin, and Genistein.

Terpenoids: α-Terpineol, Camphor, Farnesol. **Alkaloids -** Nicotine and Quinine

- 1. Organic Chemistry, I.L. Finar, Vol. I, 6th Edition and Vol. II 5th Edition, ELBS, New Delhi, 2002.
- 2. Organic Chemistry, R.T. Morrison and R.N. Boyd, 6th Edition, PHI India, New Delhi, 2011
- 3. Organic Chemistry, S.M. Mukherji, S.P. Singh, R.P. Kapoor and R. Dass, Vols, I and II, New Age International Publications, New Delhi, 2018.
- 4. Pericyclic Reactions: A Mechanistic Study, S.M. Mukherji and S.P. Singh, Macmillan India Press, New Delhi, 2012
- 5. Advanced Organic Chemistry, Jagdamba Singh and L.D.S. Yadav, Pragati Prakashan, Meerut, 2010.
- 6. Organic reactions, Stereochemistry and Mechanism, P.S. Kalasi, New Age International Publications, New Delhi, 2010.

7. Heterocyclic compounds, R.K. Bansal, New Age International Publications, New Delhi, 1999

Reference Books:

- 1. Advanced Organic Chemistry: Reactions Mechanisms and Structure, Jerry March, McGraw Hill and Kogakush., 2006.
- 2. Stereochemistry of Carbon Compounds, E. Eliel, McGraw Hill Education, Noida, 2008.
- 3. Photochemistry and Pericyclic Reactions, Jagadamba Singh and Jaya Singh, New Age International Publications, New Delhi, 2012.

Course Outcomes:

Students gain understanding of

- 1. Basic concepts of mechanisms in organic chemistry
- 2. To determine the stereochemistry of different organic molecules and various possible conformations of organic compounds
- 3. The construction of various heterocyclic rings using different organic transformations.
- 4. Different natural products with biological activity and their synthesis.

GAYATRI VIDYA PARISHAD COLLEGE FOR DEGREE AND PG COURSES (A) M.Sc. ORGANIC OF CHEMISTRY SYLLABUS I- SEMESTER PAPER IV: PHYSICAL CHEMISTRY – I (Effective from 2020-21 admitted batch)

Credits : 4		Theory : 4 Hours
Max Marks : 100	External : 80	Internal : 20

Course Objectives:

- 1. To know the knowledge of calculation of thermodynamic and kinetic parameters and learning of basic concepts in classical thermodynamics and thermodynamic processes and reactions.
- 2. The importance of statistical thermodynamics and their applications
- 3. Chemistry of surfaces of materials and different types of surface phenomenon.
- 4. Important theories and factors affecting and effect of ionic strengths on reaction rates

Unit-I

Thermodynamics

Partial molar quantity – different methods of determination of partial molar quantity – chemical potential – phase rule and its derivation - free energy change and spontaneity - Claussius–Clapeyron equation –Gibbs – Duhem equation – Duhem-Margules equation - thermodynamics of non- ideal gases – fugacity and its determination – non ideal solutions – reasons for non- ideality- activity concept – elementary concepts of excess volume and excess enthalpy – excess free energy – effect of temperature on equilibrium constant – Vant Hoff equation – Vant Hoff isotherm - Gibbs Helmholtz equation – third law thermodynamics – determination of absolute entropy.

Unit-II

Statistical thermodynamics

Ensembles (canonical and micro-canonical) - definition of distribution and micro states - thermodynamic probability - elements of statistical thermodynamics – Boltzmann distribution law – quantum statistics – Bose-Einstein and Fermi Dirac statistics - kinetic theory of gases - partition functions and their interpretation - relation between partition function and entropy, internal energy, enthalpy, free energy, pressure, translational, rotational, vibrational and electronic partition functions - heat capacity, equation of state - relation between equilibrium constant and partition function.

UNIT-III

Surface Chemistry

Surfactants and their nature – micelles and their structure - positive, negative and neutral micelles - critical micellar concentration and its determination – mixed micelles – ideal, nonideal mixed micelles – non ideality and CMC of reverse micelles – water pools and their properties –W–factor and its implications - solubilising properties of micelles - concentration effects in micellar binding of substrates and their kinetic implication - adsorption of gases on solid surfaces - Langmuir and BET isotherms – determination of surface area - structure of surfaces from photo electron spectroscopy - reactions on surfaces unimolecular and bimolecular - catalyst poisons – nature of heterogeneous catalysis

UNIT-IV

Chemical Kinetics

Empirical rate laws and their relation to mechanisms - steady state and equilibrium techniques – Lindemann's theory of unimolecular reactions - reactions in solution – effect of dielectric constant on ion-ion, ion-neutral molecule and neutral molecule - neutral molecule reactions-primary and secondary salt effects - enzyme catalysis – Michaelis-Menten mechanism – chain reactions – features – halogen reactions – decomposition of

acetaldehyde – concept of chain length – branched chain reactions – explosion limits – Linear Free Energy Relations – Hammet equation and its limitations – modification including resonance effect – Taft equation.

Course Outcomes:

- 1. The application of mathematical tools for calculation of thermodynamic and kinetic parameters and learning of basic concepts in classical thermodynamics and thermodynamic aspects of various processes and reactions.
- 2. Different aspects of statistical thermodynamics and their applications
- 3. Chemistry of surfaces of materials and different types of surface phenomenon.
- 4. Different theories and factors affecting reaction rates and effect of ionic strengths on reaction rates

- 1. Text-Book of Physical Chemistry, S. Glasstone, D. Van Nostrand Company Incorporated, 1943
- 2. Physical Chemistry, W.J. Moore, 4th Edition, Longmans, London (1963).
- 3. Physical Chemistry, G.W. Castellan, 3rd Edition, Addison-Wesley, London, 1983
- 4. Physical Chemistry, P. Atkins and J.D. Paula, 10th Edition, Oxford University Press, Oxford, 2014
- 5. Chemical Kinetics, K.J. Laidler, 3rd Edition, Pearson, New Delhi, 2003.
- 6. Principles of Physical Chemistry, B.R. Puri, L.R. Sarma and M.S. Pathania, 47th Edition, Vishal Publishing Co., Jallandhar, 2016.

SEMESTER – I PRACTICALS (Effective from 2020-21 admitted batch) LIST OF EXPERIMENTS

Credits : 3		Lab: 15 Hours
Max Marks : 75	External : 60	Internal : 15

INORGANIC CHEMISTRY

- I. Inorganic synthesis: Preparation of
 - 1. Tetraamine copper(II) sulphate
 - 2. Potassium tris- oxalate ferrate(III) trihydrate
 - 3. Tris- thiourea copper(I) sulphate
- II. Semi micro qualitative analysis of six radical mixtures (One interfering anion and one less familiar cation for each mixture)

Anions: CO₃²⁻, S²⁻, SO₃²⁻, Cl⁻, Br⁻, I⁻, NO₃⁻, SO₄²⁻, CH₃COO⁻, C₂O₄²⁻, C₄H₄O₆²⁻, PO₄³⁻, CrO₄²⁻, AsO₄³⁻, F⁻, BO₃³⁻.

Cations: Ammonium (NH₄⁺)

I group : Hg, Ag, Pb, Tl, W II group : Hg, Pb, Bi, Cu, Cd, As, Sb, Sn, Mo III group : Fe, Al, Cr, Ce, Th, Ti, Zr, V, U, Be IV group : Zn, Mn, Co, Ni V group : Ca, Ba, Sr VI group : Mg, K, Li

Text books:

- 1. Inorganic Semimicro Qualitative Analysis, V.V. Ramanujam, The National Publishing Company, Chennai, 2006.
- 2. Vogel's Qualitative Inorganic Analysis, G.Svehla, 7th Edition, Pearson Education, New Delhi, 2008.
- 3. Vogel's Text book of Quantitative Inorganic Analysis,
- J. Mendham, R.C. Denney, J.D. Barnes and M.J.K. Thomas, 6th Edition, Pearson Education, New Delhi, 2008.
- 4. Systematic Qualitative Analysis, R.M. Caven, 3rd Edition, Blackie & Son, London, 1954.

Credits : 3		Lab: 15 Hours
Max Marks : 75	External : 60	Internal : 15

ORGANIC CHEMISTRY

1. Organic synthesis: Synthesis and purification of about six organic compounds involving one or two stages.

Text books:

- 1. Vogel's Text Book of Practical Organic Chemistry, B.S. Furniss, A.J. Hannaford, P.W.G. Smith and A.R. Tatehal, Pearson Education, New Delhi, 2008.
- 2. A Laboratory Manual of Organic Chemistry, R.K. Bansal, New Age International Publishers, New Delhi, 2008.

Credits : 3		Lab: 15 Hours
Max Marks : 75	External : 60	Internal : 15

PHYSICAL CHEMISTRY

- 1. Crystal Solution Temperature of partially miscible liquids: Phenol Water system.
- 2. Effect of electrolyte (NaCl) on miscibility temperature

- 3. Determination of cell constant.
- 4. Determination of pKa value of acetic acid by conductometric method
- 5. Conductometric titration of a strong acid with strong base (HCl vs NaOH)
- 6. Conductometric titration of a weak acid with strong base (HOAc vs NaOH)

- 1. Experiments in Chemistry, D.V.Jahagirdan, 2nd Revised Edition, Himalaya Publishing House, New Delhi, 2011.
- 2. Physical Chemistry Practical, S.K. Maity and N.K. Ghosh, New Central Book Agency, Kolkata, 2012.
- 3. Practical Physical Chemistry, B. Viswanathan and P.S. Raghavan, Viva Books, New Delhi, 2012.