ADIKAVI NANNAYA UNIVERSITY
DEPARTMENT OF CHEMISTRY
FIRST SEMESTER- SYLLABUS
(With effect from 2016-17 admitted batch)

Paper- I: GENERAL CHEMISTRY-I

UNIT-1

Basic Quantum Chemistry-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 to observables; Hermitian operator- Eigen values and Eigen functions of Hermitian operator; Expansion theorems. Eigen functions of commuting operators-significance. Simultaneous measurement of properties and the uncertainty principle.

UNIT-II

Basic Quantum Chemistry-II- Wave mechanics of simple systems with constant potential energy, particle in one-dimensional box- factors influencing color transition- dipole integral, Symmetry arguments in deriving the selection rules, the concept of tunneling- particle in three -dimensional box. Calculations using wave functions of the particle in a box- Orthogonality, measurability of energy, position and momentum, average values and probabilities. Rigid rotor, Wave mechanics of systems with variable potential energy-simple harmonic oscillator- solution of wave equation- selection rules.

UNIT-III

Fundamentals of Molecular Spectroscopy-I: Microwave and IR- Spectroscopy- Rotational spectra of diatomic molecules- Rigid rotor-Selection rules- Calculations of bond length- Isotopic effect, Second order stark effect and its applications. Infrared spectra of diatomic molecules- harmonic and anharmonic oscillators- Selection rules- Overtones- Combination bands- Calculation of force constant, anharmonicity constant and zero point energy. Fermi resonance, simultaneous vibrational-rotational spectra of diatomic molecules.

UNIT- IV

Fundamentals of Molecular Spectroscopy-II: Raman and Electronic Spectra- Classical and quantum mechanical explanations- Rotational Raman and Vibrational Raman spectra. Electronic spectra of diatomic molecules- Vibrational Coarse structure- intensities of spectral lines- Frank-Condon principle- applications, Rotational Fine structure- band head and band shading. Charge transfer spectra

References/ Text books

1. Fundamentals of Molecular spectroscopy: by C.N. Banwell
2. Molecular spectroscopy: by B.K.Sharma
3. Molecular spectroscopy: by Aruldas
4. Introductory quantum mechanics: by A.K. Chandra
5. Quantum chemistry: by R.K. Prasad

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Paper- II –INORGANIC CHEMISTRY-I

UNIT-1

Structure & Bonding: Applications of VSEPR, Valence Bond and Molecular orbital theories in explaining the structures of simple molecules- role of p and d orbitals in pi bonding. Application of MO theory to square planar ($PtCl_4^{2-}$) and Octahedral complexes (CoF_6^{3-}, $Co(NH_3)_6^{3+}$). Walsh diagram for H_2O molecule.

UNIT-II

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

UNIT-III

Coordination compounds: Crystal field theory - crystal field splitting patterns in octahedral, tetrahedral, tetragonal, square planar, square pyramidal and trigonal bipyramidal geometries. Calculation of crystal field stabilization energies. Factors affecting crystal field splitting energies – Spectrochemical series – Jahn – Teller effect, nephelauxetic effect – ligand field theory. Term symbols – Russell – Sanders coupling – derivation of term symbols for various configurations. Spectroscopic ground states.

UNIT- IV

Electronic spectra of transition metal complexes: Selection rules, break down 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.

Text books:

1. Advanced Inorganic Chemistry by F.A. Cotton and G. Wilkinson, IV Edition, John Wiley and Sons, New York, 1980.
2. Inorganic Chemistry by J.E. Huheey, III Edition, Harper International Edition, 1983.
3. Theoretical Inorganic Chemistry, II Edition by M.C. Day and J. Selbin, Affiliated East-West press pvt. Ltd., New Delhi.
4. Inorganic Chemistry by Shriver and Atkins, Oxford University Press (1999).

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Paper –III, ORGANIC CHEMISTRY

UNIT – I

Nature of bonding in organic molecules and Aromaticity 15 Hrs

(A) *Electronic Effects and Reactive intermediates:*-Inductive effect, Mesomeric effect (Resonance), Hyperconjugation, Steric effect, Tautomerism, acidity and basicity of organic molecules Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes, nitrenes and arynes

(B) *Criteria of Aromaticity:*-The Energy, Structural and Electronic Criteria for Aromaticity, Relationship among the Energetic, Structural, and Electronic Criteria of Aromaticity. Huckle`s rule and MO Theory, aromaticity in benzenoid non-benzenoid compounds, Aromaticity in Charged and Fused-Ring Systems, Hetero-aromatic Systems, Annulenes: Cyclobutadiene, Benzene,1,3,5,7-Cyclooctatetraene, [10] Annulenes- [12], [14], [16] and [18] annulenes, azulenes, fulvenes, fullerenes, ferrocene, anti-aromaticity and homo-aromaticity.

UNIT – II

Stereo Chemistry & Molecular representation of organic molecules 20 Hrs

(A) Molecular Symmetry and Chirality:-Symmetry elements, Definition and classification of Stereoisomers, Enantiomer, Diastereomer, Invertomer, Homomer, Epimer, Anomer, Configuration and Conformation Configurational nomenclature: D,L and R, S nomenclature, Molecules with a single chiral center: Tetra and Tri coordinate chiral center, Molecules with two or more chiral centers; constitutionally unsymmetrical and symmetrical molecules.

(B) Geometrical Isomerism and Conformations of Cyclic Systems:- Cis-trans, E, Z- and Syn & anti nomenclature, Methods of determining configuration of Geometrical isomers using physical, spectral and chemical methods, Stability, Cis-trans inter conversion. Conformations of cyclobutane, cyclopentane, cyclohexane, mono and disubstituted cyclohaxanes.

(C) Prochirality and Prostereoisomerism:- Homotopic ligands and faces; enantiotropic ligands and faces; diastereotopic ligands and faces; nomenclature of enantiotopic ligands and faces (Pro-R, Pro-S, Re, Si carbonyl compounds and Alkenes)

(D) Stereoisomerism in molecules without chiral Center -Axial chirality Allenes, Alkylidene cycloalkanes, spiranes, nomenclature. *Atropisomerism:* Biphenyl derivatives, nomenclature. *Planar chirality*: Ansa compounds, paracyclophanes, trans-cyclooctene and Helicity.

UNIT – III

Heterocyclic compounds 15 Hrs

Importance of heterocyclic compounds as drugs. Nomenclature of heterocyclic systems based on ring size,number and nature of hetero atoms. Chemistry of heterocyclic compounds, synthesis and reactivity of the following systems: Quinoline, Isoquinoline, Indole, Pyrazole, Imidazole, Oxazole, Isoxazole, Pyridazine, py.rimidine and Pyrazine.

UNIT - IV

Chemistry of some typical natural products (Alkaloids and Terpenoids) 10 Hrs

A study of the following compounds involving their isolation, structure elucidation, synthesis and biogenesis of

Alkaloids; Atropine, Nicotine, and Quinine.

Terpenoids: α- Terpeneol, α-Pinene and Camphor.

Books Suggested:

1. Advanced Organic Chemistry-Reactions, Mechanism and structure, Jerry March, 6th Ed. (John Wiley & Sons).
2. Organic Chemistry, Paula Yurkanis Bruice, 4th Ed. (Printice Hall)
3. Organic chemistry-Clayden J. (Oxford)
4. Organic Chemsitry, Wade, L.G. Jr. 5th Ed. (Pearson)
5. Advanced Organic Chemistry: Reactions and mechanisms, Miller Bernard & Other, 2nd Ed. (Pearson)
6. Mechanism and Theory in Organic Chemistry, Thomas H. Lowry, Kathleen S. Richardson, Harper & Row, (Publishers, Inc.).
7. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, 6th Ed., (Longman).
8. Reaction Mechanism in Organic Chemistry, P.S. Kalsi, 2nd Ed. (New Age International).
9. Organic Chemistry, R. T. Morrison and R. N. Boyd (Prentice-Hall)
10. Stereochemistry to Organic Compounds, E.L. Eliel (John Wiley).
11. Stereochemistry, P.S. Kalsi, 5th Ed. (New Age International).
12. Organic Chemistry Structure and Reactivity, Ege Seyhan, 3rd Ed. (AITBS)
13. Heterocyclic Chemistry, J.A.Joule, K. Kills and G. F. Smith, Chapman and Hall
14. Heterocyclic Chemistry, T.L.Gilchrist, Longman Scientific Technical
15. Heterocyclic Chemistry, Raj.K. Bansal.
16. An Introduction to the Heterocyclic Compounds, R. M. Acheson, John Wiley.

REFERENCE BOOKS:

1. Chemistry of Natural Products, K.W.Bentley
2. Stereochemistry of carbon compounds by E.Eliel, John Wiley & Sons, Inc.
3. Stereochemistry to Organic Compounds, D. Nasipuri, 2nd Ed. (New Age International).
4. Chemistry of Natural products by R.S. Kalsi Kalyani Publishers. 1983.

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Paper – IV- PHYSICAL CHEMISTRY-I

UNIT-I:

Thermodynamics-I: Concepts of partial molar properties – partial molar volume and its significance; Determination of partial molar volume: Graphical method, intercept method and apparent molar volume method. Partial molar free energy, chemical potential, Variation of chemical potential with T and P. Gibbs-Duhem equation-derivation and significance. Phase equilibrium- Derivation of phase rule from the concept of chemical potential. *Ideal solutions* - Thermodynamic properties of ideal solutions mixing quantities; Vapour pressure-Raoult's law; Thermodynamic properties of ideally dilute solutions. Vapour pressure- Henry's law.

Non-ideal systems -Concept of fugacity, fugacity coefficient. Determination of fugacity; Non ideal solutions. Activities and activity coefficients; Standard-state conventions for non ideal solutions; Determination of activity coefficients from vapour pressure measurements. Activity coefficients of non-volatile solutes using Gibbs-Duhem equation. Chemical equilibrium- effect of temperature on equilibrium constant- Van'tHoff equation

UNIT-II:

Micelles and Macro molecules: Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization- phase separation and mass action models, Solubilization, micro emulsion, reverse micelles.

Polymer- definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of free radical polymerization. Molecular mass- Number and mass average molecular weight, molecular weight determination-End group analysis, Osmometry, viscometry, ultracentrifugation and light scattering methods.

UNIT-III:

Chemical Kinetics: Theories of reaction rates- Collision theory- Limitations, Transition state theory. Effect of ionic strength - Debye Huckel theory-Primary and secondary salt effects; Effect of dielectric constant, effect of substituent, Hammett equation-limitations, Taft equation; Prediction of rate constants- Consecutive reactions, parallel reactions, opposing reactions (Uni molecular steps only, no derivation). Specific and general acid-base catalysis; Skrabal diagram; Fast reactions- different methods of studying fast reactions- flow methods, relaxation methods- temperature jump and pressure jump methods.

UNIT-IV:

Photochemistry: Electronic transitions in molecules, Franck-Condon principle. Electronically excited molecules- singlet and triplet states, spin-orbit interaction. Quantum yield and its determination; Actinometry - ferrioxalate and uranyl oxalate actinometers-problems. Derivation of fluorescence and phosphorescence quantum yields. Quenching effect- Stern Volmer equation. Photochemical equilibrium and delayed fluorescence - E type and P type. Photochemical primary processes, types of photochemical reactions-photodissocoation, addition and isomerisation reactions with examples.

Books:

1. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press.
2. Physical Chemistry by G.W. Castellon, Narosha Publishing House
3. Physical Chemistry by W.J.Moore, Prentice Hall
4. Thermodynamics for Chemists, Samuel Glasstone
5. Chemical Kinetics by K.J.Laidler, McGraw Hill Pub.
6. Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson.
7. Polymer Chemistry by Billmayer
8. Introduction to Polymer Science, V.R. Gowriker, N.V.Viswanadhan and J. Sreedhar., Wiley Easter.
9. Micells, Theoretical and applied aspects, V.Morol, Plenum publishers.

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LABORATORY WORK (6 hrs/week)

INORGANIC CHEMISTRY - I

I. *Inorganic Synthesis: Preparation of*

(i) Tetraamminecopper(II) sulphate

(ii) Potassium tris-oxalato ferrate(III) trihydrate

(iii) 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: CO_3^{2-} , S^{2-} , SO_3^{2-} , Cl^- , Br^- , I^- , NO_3^- , SO_4^{2-}, CH_3COO^-
$C_2O_4^{2-}$, $C_4H_4O_6^{2-}$, PO_4^{3-} , CrO_4^{2-}, AsO_4^{3-}, F^- , BO_3^{3-}

Cations : Ammonium (NH_4^+)
1^{st} group: Hg, Ag, Pb, Tl, W
2^{nd} group: Hg, Pb, Bi, Cu, Cd, As, Sb, Sn, Mo
3^{rd} group: Fe, Al, Cr, Ce, Th, Ti, Zr, V, U, Be
4^{th} group: Zn, Mn, Co, Ni
5^{th} group: Ca, Ba, Sr
6^{th} group: Mg, K, Li

ORGANIC CHEMISTRY -I

Preparation, recrystallization, and determination of melting point & yield of the following compounds:

(i)	Aspirin,	(ii)	Nerolin,	(iii)	Chalcone,
(iv)	*p*-Nitro acetanilide,	(v)	2,4,6- Tribromoaniline,	(vi)	*m*-Dinitrobenzene,
(vii)	Phthalimide,	(viii)	Diels-Alder adduct.		

Books Suggested

1. Vogel's Text Book of Quantitative Chemical Analysis, J. Mendham, R. C. Denney, J. D. Barnes and M. J. Thomas, 4th & 6th Ed. (Pearson Education Asia).

2. Vogel's Text Book of Practical Organic Chemistry, B.S. Furniss, A.J. Hannaford, P.W.G. Smith, A.R. Tatchell, 5 Ed. (Longman Scientific & Technical)

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PHYSICAL CHEMSITRY-I

1. Determination of critical solution temperature of phenol-water system.
2. Effect of added electrolyte on the CST of phenol-water system.
3. Conductometric titration of Strong acid versus Strong base
4. Dissociation constant of weak acid (CH_3COOH) by conductometric method.
5. Conductometric titration of Weak acid vs Strong base.
6. Determination of cell constant
7. Adsorption of acetic acid on animal charcoal or silica gel.
8. Acid-catalyzed hydrolysis of methyl acetate
9. Determination of partial molar volume of solute $-H_2O$ system by apparent molar volume method.