M. Sc. Semester -I

CHE401 Inorganic Chemistry

Unit 1 - Quantum theory and Atomic Structure

Postulates of quantum mechanics, setting up of different observables, eigen value of angular momenta and commutation relations, step-up and step-down operators, angular momenta in many electron atoms.

Schroedinger wave equation and applications: particle on a ring and the simple harmonic oscillator.

H-atom wave functions, solutions of \( R_{(r)} \), \( \theta_{(\theta)} \) and \( \phi_{(\phi)} \) equations, quantum numbers, angular and radial wave function, shapes of the orbitals, angular momentum of inner quantum number \( j \), physical interpretation of hydrogenic orbitals; space quantization of electronic orbits; electron spin.

Approximation methods: Variation method and application to H atom. Perturbation theory (first order and non-degenerate, application to the Helium atom.

Unit 2 - Symmetry and Group Theory

Representation of groups–some properties of matrices & vectors, representation of groups, the Great orthogonality theorem and its consequences, character table, wave functions as basis for irreducible representations, direct product, identifying non-zero matrix elements.

Unit 3 - Magnetochemistry

Magnetic susceptibility and basic derivation of diamagnetic susceptibility, pascal constant and its utility, Curie law and Curie-Weiss law, antiferromagnetism and ferromagnetism. Types of antiferromagnetism, antiferro magnetic exchange pathway:

Direct –metal- metal interaction and Indirect-atom exchange i.e. super exchange mechanism.

Unit 4 - Bio-inorganic Chemistry

Metalloporphyrins (enzymes) definition, hemoglobin and myoglobin, cytochrome, vitamin B_{12} (cyano cobalamin), zincmetallo enzymes, nitrogen fixation, essential and trace elements in biological system, biochemistry of non metals K, Na pump (action of bath ions), toxic metals and their toxicity.

Co-ordination compounds in medicine

Chelation therapy, gold compounds and rheumatoid arthritis, anticancer drugs –platinum complexes, gold complexes, metalloccenes etc, antimicrobial agents, metal complexes as radiodiagnostic agents, magnetic resonance imaging.
References:
1. Introduction to Quantum Chemistry, A. K. Chandra, Tata MacGraw Hill
2. Quantum Chemistry, Ira N. Levine, Prentice Hall
5. D. A. McQuarrie Quantum Chemistry, OUP 1983
17. Inorganic Reaction Mechanisms, M. L. Tobe, Nelson Pub
25. Elements of Magnetochemistry, Dutta and Syamal, 1993
1. Semi-microqualitative analysis of 15 mixtures, each having six radicals including less familiar elements (Mo, W, Li, Th, V, Zr, Ce, Be, Ti) and one insoluble compounds.

References
M.Sc. SEMESTER - I
CHE402 Organic Chemistry

Unit-1

(A) Elimination Reaction


(B) Nucleophilic Substitution Reaction

Mixed SN₁, SN₂ and SET mechanism.
Nucleophilic substitution at (a) Allylic carbon (Allylic rearrangements), (b) An Aliphatic trigonal carbon (the tetrahedral mechanism) and at (c) A Vinyl carbon. Participation of Neighboring groups in Nucleophilic substitution by (a) Carboxylate anion (b) Halogen atoms (c) Hydroxyl groups (d) Acetoxy group (e) Phenyl group (f) RS group (g) Participation by π-bond.

Unit-2

(A) Aromaticity

Aromaticity, aromatic character, Frost circle diagram for cyclobutadiene, benzene and others. Resonance and chemical stabilization-aromatic character based on NMR criteria, Huckels rule, energy level of π molecule orbital, Huckels molecular orbital(HMO) method, MO of simple organic systems such as ethene, allyl and butadiene Aromaticity in benzenoid and non-benzenoid compounds and charged rings, annulenes, fulvenes, azulenes, antiaromaticity and homoaromaticity.

(B) Acid base concept, pKa, Hammet equation, Concept of hindered base, The effect of structure on the strength of acids and bases.
Unit - 3

(A) Reactive intermediates
   (1) Carbocations (classical and non classical) stability, structure, generation and fate
   (2) Carbanions- stability, structure, generation and fate of carbanions
   (3) Carbenes-stability and structure, the generation and fate of carbenes.
   (4) Free radicals: stability, structure, generation and fate of free radicals, NBS
   (5) Nitrene : stability, structure, generation, reaction

(B) Rearrangements:
   General mechanistic considerations, nature of migration, migratory aptitude, and memory effects in respect of following.
   (1) Carbon to Carbon migration of R, H and Ar
      (i) Pinacol- Pinacolone rearrangement
      (ii) Favorstskii rearrangement
   (2) Carbon to Nitrogen migrations:
      (i) Curtius rearrangement
      (ii) Schmidt rearrangement
   (3) Carbon to oxygen migration of and Ar
      (i) Baeyer- villiger rearrangement
      (ii) Rearrangement of hydroperoxide

Unit - 4
Stereo Chemistry
   Optical and geometrical isomerism, origin of chirality and chiral centre, axis and plane, helicity, Enantiotopic and diastereotopic atoms, groups and faces, prochiral centre, biphenyl, allenes, spirans, compounds containing chiral nitrogen and sulfur, stereospecific and stereoselective synthesis, dynamic resolution.
References:
2) Carbenes, nitrenes and arynes, T.L. Gilchrist and C.W. Rees.
9) Physical Organic Chemistry by Jack Hynes,(plenum publication)
Preparation of organic compounds:

i) Nitration
ii) Bromination
iii) Acylation
iv) Reduction
v) Oxidation
vi) Condensation reaction
vii) Diazotization reaction
viii) Friedl-Craft’s reaction
ix) Cannizzaro reaction
x) Aldol condensation

Quantitative Estimations

a. Estimation of ester + acid
b. Estimation of formaldehyde
c. Estimation of glycine
d. Estimation of amide + acid
M. Sc. - Semester – I (PRACTICALS)
CHE405PR  Organic Chemistry

References:
1. A text book of practical organic chemistry – A. I. Vogel
2. Practical organic Chemistry – Mann and Saunders
3. A handbook of quantitative and qualitative analysis – H. T. Clarke
M.Sc. Semester I

CHE403 Physical Chemistry

Unit I - Chemical thermodynamics:
Nernst heat theorem and its applications to gaseous system, third law of thermodynamics and its applications to evaluate absolute entropies of solids, liquids and gases; partial molar quantities and their determination, Gibbs-Duhem equation, chemical potential, chemical potential of idea gases and solutions, Raoult’s law, real solutions, free energy and solutions, activity and activity coefficients, methods of determination of activity and activity coefficients, fugacity of gases and liquids and methods of its determination.
Non equilibrium thermodynamics-basic concepts.

Unit II - Chemical Kinetics:
Unimolecular reactions, chain reactions and branched chain reactions, explosion limits, chain reaction between hydrogen and bromine, theory of absolute reaction rates, kinetic isotope effect.
Enzyme catalyzed reactions, mechanism, kinetics and some examples.

Unit III - Solid state chemistry:

Unit IV - Surface chemistry:
Physical and chemical adsorption, BET and HJ equations, heat of adsorption, determination of surface area of adsorbents, surface tension, Gibb’s equation, surface active agents, micellisation, critical micellar concentration (cmc), detergency.
M. Sc. Semester I- References: Theory

(1) Textbook of physical chemistry – W.J.Moore
(2) Textbook of physical chemistry – Glasstone
(3) Textbook of physical chemistry – P.Atkins
(4) Advanced physical chemistry – Surdeep Raj
(5) Advanced physical chemistry – J.N.Gurtu, A.Gurtu
(6) Thermodynamics for chemists – Glasstone
(7) Physical chemistry – S. Castellian
(8) Thermodynamics of non equilibrium processes- Karapitianeh
(9) Chemical Kinetics- Laidler
(10) Chemical Kinetics – Frost and Pearson
(11) Solid state chemistry – H.Keer
(12) Solid state chemistry- Hannay
(13) Chemistry of solids – Azaroff
(14) Surface chemistry – Adamson
(15) Surface chemistry – Osipov
M.Sc. Semester I - Practicals

CHE406PR Physical Chemistry

I. Conductometry
   1. Titration of mixture of strong acid and weak acid with strong base (HCl + HAC against NaOH)
      Titration of mixture of strong acid and weak acid with weak base (HCl + HAC against H₄OH)
   2. Solubility product of sparingly soluble salts – PbSO₄ & BaSO₄

II. Potentiometry
   1. Titration of mixture of strong (HCl) and weak (HAC) acid with NaOH / NH₄OH and find the strength of the acids in mixture.
   2. Solubility product of silver halides.

III. pHmetry
   1. Titration of mixture of strong (HCl) and weak (HAC) acid with NaOH / NH₄OH and find the strength of the acids.
   2. Titration of mixture of bases (Na₂CO₃ & NaHCO₃) with standard HCl and find the concentration of bases.

IV. Adsorption and kinetics
   1. Hydrolysis of esters
   2. Reaction between K₂S₂O₈ and KI.

V. Distribution method
   1. Distribution of acetic acid between H₂O and butanol.
   2. Distribution of HAC between H₂O and CHCl₃ / CCl₄.
   3. Distribution of I₂ between H₂O and CCl₄.
References:

(1) Practical physical chemistry – J.B. Yadav
(2) Practicals in physical chemistry – P.S. Sindhu
(3) Experimental physical chemistry – R.C. Das, B. Behera
(4) Experiments in physical chemistry – P.H. Parsania, F. Karia
M.Sc. Semester I
CHE404 Analytical Chemistry

UNIT-1
Analytical Objectives, Data Handling and Good Laboratory Practice (GLP)
Scope of analytical science and its literature, qualitative and quantitative analysis, ways to express accuracy and precision, types of errors and their causes; significant figures, control charts, confidence limit, test of significance, rejection of a result- the Q-test. GLP- standard operating procedures, quality assurance and quality control, validation of analytical methods.

UNIT-2
Sampling and Calibration Methods
Sampling and sample preparation, general steps in chemical analysis, calibration of glass wares. Finding the best straight line-least square regression, correlation coefficient; Calibration curves, standard addition technique and internal standards. Chemical concentrations.

UNIT-3
Fundamentals of Spectrophotometry

UNIT-4
Applications of Spectrophotometry
Analysis of mixture-resolved and unresolved spectra, measurement of equilibrium constant: Scatchard Plot; Stoichiometry-method of continuous variation- the Jobs plot. Photometric titrations.

M.Sc. Semester I
CHE404 Analytical Chemistry- Theory

Reference Books
M.Sc. Semester I
Analytical Chemistry-CHE406PR -Practicals

2. Calibration of pH meter, conductometer and potentiometer.
3. Determination of nicotine in tobacco (non-aqueous titration).
4. Determination of available chlorine in bleaching powder.
5. Determination of vitamin C in orange juice/amlac.
6. Determination of acetic acid in vinegar.
7. Determination of sodium carbonate and sodium bicarbonate in washing soda.
8. Determination of ascorbic acid in vitamin C tablets.
10. Determination of total dissolved solids in water samples.
11. Determination of sulphate in water sample.
12. Determination of chloride in water sample.

References: