

## 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.

Schrodinger 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, antiferromagnetic 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<sub>12</sub> (cyano cobalamin), zinc metallo 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, metallocenes etc, antimicrobial agents, metal complexes as radiodiagnostic agents, magnetic resonance imaging.

## **CHE401 Inorganic Chemistry**

### **Semester I – Theory**

#### **References:**

1. Introduction to Quantum Chemistry, A. K. Chandra, Tata MacGraw Hill
2. Quantum Chemistry, Ira N. Levine, Prentice Hall
3. Quantum Chemistry by R. K. Prasad, New Age International Publishers (1985)
4. Elementary Quantum Chemistry by D. L. Pilar, Mc Graw Hill Book Co, New York (1968)
5. D. A. McQuarrie Quantum Chemistry, OUP 1983
6. M. W. Hanna, Quantum Mechanics in Chemistry, The Benjamin Pub.
7. Molecular Quantum Mechanics, Third Edition, P. W. Atkins and R.S. Friedman
8. Group theory and symmetry in chemistry, L. H. Hall(McGraw Hill)
9. F. A. Cotton, Chemical Applications of Group theory, Wiley Eastern 2<sup>nd</sup> Edn.1992
10. V. Ramkrishnan & M. S. Gopinadhan, Group theory in Chemistry Vishal Pub.1996.
11. Inorganic Chemistry, Third Edition, Alan G. Sharpe
12. Theoretical Inorganic Chemistry, M. C. Day, J. Shellin
13. Chemistry, Fifth Edition, John E. McMurry, Robert C. Fay
14. Hermann Dugas, Bioorganic Chemistry, A Chemical Approach to Enzyme Action, Springer International Edition
15. An Introduction to Theoretical Chemistry, Jack Simons, Cambridge
16. Progress in inorganic Chemistry, Vols 18 and 38 ed. J. J. Lippard, Wiley
17. Inorganic Reaction Mechanisms, M. L. Tobe, Nelson Pub
18. Inorganic Chemistry, K. F. Purcell and J. C. Kotz.
19. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Bers
20. Bioinorganic Chemistry, I. Bertini, H. B. Gray and S. J. Lippard
21. Principals of Bioorganic Chemistry, S. J. Lippard and J. M. Berg, University Science Books.
22. Bioinorganic Chemistry, I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, University Science Books.
23. Inorganic Biochemistry vols I and II ed. G. L. Eichhorn, Elsevier
24. Introduction to Magnetochemistry, Alan Earnshaw, 1968
25. Elements of Magnetochemistry, Dutta and Syamal, 1993

**M. Sc. Semester I- Practicals**  
**CHE405PR Inorganic Chemistry**

**Semester –I Practicals ( Inorganic Chemistry) CHE405PR**

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.

**M. Sc. Semester I- Practicals**  
**CHE405PR Inorganic Chemistry**

**References**

1. Vogel's Qualitative Inorganic Analysis, Revised by G Svehla, Sixth Edition, Longman, 1987

**M.Sc. SEMESTER - I**  
**CHE402 Organic Chemistry**

**Unit-1**

**(A) Elimination Reaction**

The E<sub>1</sub>, E<sub>2</sub>, E<sub>1</sub>CB mechanism, stereochemistry. Orientation of the double bond *syn* and *anti* eliminations. Reactivity- effects of substrate structures, attacking base, leaving group and medium. Mechanism and orientation in pyrolytic *syn* eliminations – Chugaev and Cope eliminations.

**(B) Nucleophilic Substitution Reaction**

Mixed SN<sub>1</sub>, SN<sub>2</sub> 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  $\pi$ -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  $\pi$  molecular orbitals, 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, pK<sub>a</sub>, Hammett 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) Favorskii 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.

**M.Sc. SEMESTER – I**  
**CHE402 Organic Chemistry : Theory**

**References:**

- 1) Advanced Organic Chemistry, Reactions Mechanisms and Structure , J. March, 6<sup>th</sup> Edition, John Wiley.
- 2) Carbenes, nitrenes and arynes, T.L. Gilchrist and C.W. Rees.
- 3) Guidebook to Mechanism in Organic Chemistry by Peter Sykes, 6<sup>th</sup> Edition, Prentice Hall.
- 4) Advanced Organic Chemistry Part A: Structure and Mechanism and Part B: Reaction and synthesis ,Francis A. Carey, Richard J. Sundberg, 5<sup>th</sup> Edition, Springer .
- 5) Organic Chemistry, Johnathan Clayden, Nick Greeves, Stuart Warren, 1<sup>st</sup> Edition, Oxford University Press.
- 6) Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, 3<sup>rd</sup> Edition, Blackie Academic and Professional.
- 7) Stereo Chemistry , P.S. Kalsi , New Age Publications.
- 8) Reagents in Organic Synthesis- Fieser and Fieser, John Wiley.
- 9) Physical Organic Chemistry by Jack Hynes,(plenum publication)
- 10) Organic Chemistry, T.W. Graham Solomons and Graig B. Frymes, John Wiley and Sons.
- 11) Organic Chemistry, F. A. Carey, McGraw Hill Edition.
- 12) General Organic Chemistry Sachin Kumar Ghose, New Central book agency.
- 13) Organic Chemistry Vol 1-2 I.L.Finar 5<sup>th</sup> edition,ELBS.

**M.Sc. - Semester – I (PRACTICALS)**  
**CHE405PR Organic Chemistry**

**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
4. Comprehensive Practical Organic Chemistry : Qualitative Analysis V K Ahluwalia & S. Dhingra.
5. Comprehensive Practical Organic Chemistry : Preparations and Quantitative Analysis V K Ahluwalia & R. Aggarwal Universities Press.
6. An Advance Course in practical Chemistry, A K. Nad, B. Mahapatra and A. Ghoshal.



# 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 ideal 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:**

Bonding in solids and electronic structure in solids, band theory-metals, semiconductors and insulators, defects in crystals, calculation of Schottky and Frenkel defects using statistical method, non stoichiometry, solid electrolytes, diffusion in solids, electrical conductivity in solids, super conductivity, perovskites.

### **Unit IV- Surface chemistry:**

Physical and chemical adsorption, BET and HJ equations, heat of adsorption, determination of surface area of adsorbents, surface tension, Gibbs' 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. Castellan
- (8) Thermodynamics of non equilibrium processes- Karapitaneh
- (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 H<sub>4</sub>OH)
2. Solubility product of sparingly soluble salts – PbSO<sub>4</sub> & BaSO<sub>4</sub>

### II Potentiometry

1. Titration of mixture of strong (HCl) and weak (HAC) acid with NaOH / NH<sub>4</sub>OH and find the strength of the acids in mixture.
2. Solubility product of silver halides.

### III pH metry

1. Titration of mixture of strong (HCl) and weak (HAC) acid with NaOH / NH<sub>4</sub>OH and find the strength of the acids.
2. Titration of mixture of bases (Na<sub>2</sub>CO<sub>3</sub> & NaHCO<sub>3</sub>) with standard HCl and find the concentration of bases.

### IV Adsorption and kinetics

1. Hydrolysis of esters
2. Reaction between K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> and KI.

### V Distribution method

1. Distribution of acetic acid between H<sub>2</sub>O and butanol.
2. Distribution of HAC between H<sub>2</sub>O and CHCl<sub>3</sub> / CCl<sub>4</sub>.
3. Distribution of I<sub>2</sub> between H<sub>2</sub>O and CCl<sub>4</sub>.

# **M.Sc. Semester I - Physical Chemistry Practicals- CHE406PR**

## **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**

Properties of light, absorption of light, interaction of light with matter and origin of spectra. The spectrophotometer- calibration, sources of light, monochromators and detectors. Beer's law in chemical analysis, photometric accuracy- Ringbom Plot, derivative spectrophotometry, optical rotatory dispersion and circular dichroism.

### **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**

1. "Quantitative Chemical Analysis" by Daniel C. Harris, 5<sup>th</sup> Edition, W.H. Freeman and Company, New York.
2. "Analytical Chemistry" by Gary D. Christian, 6<sup>th</sup> Edition, John Wiley and Sons Inc. New Jersey.
3. "Principles of Instrumental Analysis" by Douglas A. Skoog, 3<sup>rd</sup> Edition, Holt-Saunders International Edition.
4. "Instrumental Methods of Chemical Analysis" by Galen W. Ewing, 4<sup>th</sup> Edition, International Student Edition.

**M.Sc. Semester I**  
**Analytical Chemistry-CHE406PR -Practicals**

1. Calibration of glass wares and balance.
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/amlá.
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.
9. Determination of calcium and magnesium in water sample.
10. Determination of total dissolved solids in water samples.
11. Determination of sulphate in water sample.
12. Determination of chloride in water sample.

**M.Sc. Semester I**  
**Analytical Chemistry-CHE406PR -Practicals**

**References:**

1. Analytical Chemistry Practice, John H. Kennedy, Saunders College Publishing, Second Edition 1990.
2. Vogels Textbook of Quantitative Chemical Analysis, 6<sup>th</sup> Edition, 2002.