# M. Sc. Semester II

Inorganic Chemistry-**CHE407**

**Unit I- Chemical Bonding**

The method of linear combination

VSEPR, Walsh diagrams(tri-and penta- atomic molecules), $d_\pi - p_\pi$ bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

Simple Huckel theory of linear conjugated systems, simple Huckel theory of the cyclic conjugated system and aromaticity, self consistent filed method, valence state ionization potentials, Pariser-Parr-Pople appoximation.

Band theory of solids, Fermi level, electrical properties, insulators, semiconductors and superconductors (properties).

**Unit 2- Application of symmetry**

Application of symmetry to hybrid orbital, molecular orbitals, hybridization schemes for $\sigma$ orbitals, $\pi$ bonding and molecular orbital for ABn type of molecules.

Application of symmetry to molecular vibrations, interpretation of IR and Raman spectral data.

**Unit 3-Organometallic Compounds**

Organometallic compounds of transition elements, stability of metal carbon bond in complexes. Synthesis, uses and structure of organometallic compounds of $\pi$ bonding organic ligands, 2-electron ligands, olifinic and acetylinic complexes, compound with 3 electron ligand – allylic complexes, compounds. With 4- electron ligands butadiene complexes, $n^4$ complexes of cyclopentadiene, compounds with 5 electron ligands – cyclopantadionyl, compounds with 6 electron ligands, $n^6$ complexes of benzene and its derivatives.

Role of organometallic compounds in catalytic reaction.

**Unit 4 – Reaction Mechanism**

Mechanism of substitution reaction in square planar complexes. Kinetics of substitution reaction of platinum (II) complexes

Effect of leaving group, effect of charge, steric effect, solvent effect, effect of nucleophile, effect of tempeature and other effects.

Oxidation-Reduction reaction, electron transfer, tunnelling effect, Marcus –Hush theory, one and two electron transfer inner sphere and outer sphere, effect of ions on rate, electron transfer through extended bridges, unstable oxidation states, hydrated electron.

# M. Sc. Semester –II

## CHE407 (Inorganic Chemistry)- 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. D. A. McQuarrie Quantum Chemistry, OUP 1983
5. M. W. Hanna, Quantum Mechanics in Chemistry, The Benjamin Pub.
6. Lectures on Chemical Bonding and Quantum Chemistry, S. N. Datta, A Prism Book
7. Group theory and symmetry in chemistry, L. H. Hall(McGraw Hill)
8. Coulson's Valence, R. McWeeny, ELBS
9. F. A. Cotton, Chemical Applications of Group theory, Wiley Eastern 2nd 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. An Introduction to Theoretical Chemistry, Jack Simons, Cambridge
15. Progress in inorganic Chemistry, Vols 18 and 38 ed. J. J. Lippard, Wiley
16. Mechanism of Inorganic Reactions, F. Basolo and R. G. Persons, Wiley Pub
17. Reaction Mechanism of Coordination Compounds, C. H. Langford and H. B. Gray
18. Inorganic Reaction Mechanisms, M. L. Tobe, Nelson Pub
19. Inorganic Chemistry, K. F. Purcell and J. C. Kotz.
20. Principles of Bioinorganic Chemistry, S. J. Lippard and J. M. Bers
21. Mehrotra R. C. and Singh A. Organo Metallic Chemistry, Willey Eastern Ltd., New Delhi
22. Coates G. E. Green MIH Wade, K and Aylett B. J. Organo Metallic Comounds Chapman and Hall, London

# M. Sc. Semester II- Practicals

**CHE411PR (Inorganic Chemistry)**

**Semester –II Practicals (Inorganic Chemistry) CHE411PR**

1. Preparation and determination of purity of double and complex salts. At least ten preparations should be done.
2. Colourimetric estimation of any five out of Cu, Mn, $NO_2$, Ni, P, Fe, V, Ti, Cr, Co.

# M. Sc. Semester II- Practicals

**CHE411PR (Inorganic Chemistry)**

**References**

1. Vogels Textbook of Quantitative Chemical Analysis, $6^{th}$ Edition, 2002.
2. Advanced Practical Inorganic Chemistry, Gurdeepraj, Goel Publishing House, 2001.
3. An Advanced Course in Practical Chemistry, A.K. Nad, B. Mahapatra, A. Ghosal, New Central Book Agency, 2004

## M.Sc. SEMESTER II

## CHE408 Organic Chemistry

**Unit-1**

**Spectroscopy**

**1)** 13 CNMR : General considerations, chemical shift ( aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants.

**2)** Mass spectroscopy : Introduction, ion production, EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectroscopy.

**3)** Examples of mass spectral fragmentation of organic compounds, NMR, IR, UV with respect to their structure determination.

**Unit - 2**

**(A) Photochemistry:**

(1) Photochemical reactions: Principles of energy transfer, electronic excitation and molecular orbital view of excitation, excited states and fate of excited molecules (modified Jablonski diagram), Photosensitization.

(2) Photochemistry of carbonyl compounds: Representation of excited states of ketones, photoreduction Norrish typeI& Π reactions, Reactions of cyclic Ketone, oxetane formation (Paterno-Buchi reaction)

(3) Di-π methane rearrangement, Dienone photochemistry, cis-trans isomerisation and photochemistry of conjugated olefins.

**(B) Chemistry of Heterocycles**

(1) Nomenclature of heterocycles : Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles. General chemical behavior of aromatic heterocycles.

(2) Five-membered and benzo fused five member heterocycles : Oxazole, Isoxazole, Thiazole, Pyrazole, Imidazole, Benzothiazole and Benzimidazole.

(3) Six membered and benzofused six membered heterocycles : Pyrazine, Pyridazine, Pyrimidine, Cinnoline, Quinazoline, Quinoxaline, Phenoxaline.

**Unit - 3**

**Name reactions :** General nature, method, mechanism and synthetic applications of the following reactions:

(i) Vilsmeier-Haack reaction
(ii) Mitsunobu reaction
(iii) Suzuki reaction
(iv) Buchwald Hartwing reaction ( cross coupling)
(v) Sonogarshira coupling
(vi) Stobbe condensation
(vii) Jones oxidation
(viii) Swern oxidation reaction
(ix) Michael addition
(x) Darzen's glycidic ester synthesis
(xi) Mannich reaction
(xii) Dickmann reaction
(xiii) Birch reduction
(xiv) Witting reaction
(xv) Knoevanagel reaction

**Unit-4**

**Reagents in organic synthesis** : Mechanism selectivity and utility of following reagents:

(i) Gilman's reagent-Lithium dimethylcuprate
(ii) Lithium diisopropylamide (LDA)
(iii) Dicyclohexyl carbodiimide (DCC)
(iv) 1,3 – Dithiane (Umpolung reagent)
(v) Dess- Martin periodinane
(vi) Bakers yeast
(vii) Diisobutylauminium hydride( DIBAL –H)
(viii) Sodium cyanoborohydride (NaBH3(CN))
(ix) Grignard reagents
(x) Sodium borohydride
(xi) DDQ
(xii) n-Butyl lithium
(xiii) Phase transfer catalysis : Quaternary ammonium and phosphonium salts, crown ethers.

## M.Sc. SEMESTER II - Theory

## CHE408 Organic Chemistry

## References


1) Modern Synthetic Reactions, H.O.House, W.A. Benjamin.
2) Principles of Organic Synthesis, R.O.C. Norman and J.M. Coxon, 3rd Edition, Blackie Academic and Proffessional.
3) Spectrometric Identification of Organic Compounds by Robert M. Silverstein, 7th Edition ,Wiley.
4) Mass Spectrometry – A Textbook Jurgen Gross, 1st Edition , 2002, Springer – Verlag Berlin Heidelberg.
5) Introductory Photochemistry, A.Cox and T.Camp, McGraw Hill.
6) Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson.
7) Organic Photochemistry, J. Coxon and B. Halton, 2nd Edition , Cambridge University Press.
8) Stategic Applications of Named Reactions in Organic Synthesis, Laszlo Kurti and Barbara Czak, 1st Edition ,Acedemic Press.
9) Name Reactions and Reagents in Organic Synthesis, Bradford P. Mundy, Michael G. Ellerd , Frank G. Favaloro, 2nd Edition, Wiley – Interscience.
10) Name Reactions. A Collection of Detailed Reaction Mechanisms., Jie Jack Li, 3rd Edition , Springer.
11) Heterocyclic Chemistry, volume 1-3, R.R. Gupta, M. Kumar and V. Gupta, Springer- Verlag.
12) Heterocyclic Chemistry, J.A. Joule, K.Mills, and G.F. Smith, 3rd Edition, Chapman and Hall.
13) Heterocyclic Chemistry, T.L. Gilchrist, Longman Scientific Technical.
14) Contemporary Heterocyclic Chemistry, G.R. Nikome and W.W. Poudler, Wiley.
15) Comprehensive Heterocyclic Chemistry, A.R. Kartizky, and C.W. Rees.
16) Encyclopedia of Reagents for Organic Synthesis, Leo A. Paquette, David Crich and Phillip L. Fuchs, John Wiley and Sons Inc.
17) Organic Chemistry, T.W. Graham Solomons and Graig B. Frymes, John Wiley and Sons.
18) Organic Chemistry, F. A. Carey, McGraw Hill Edition.
19) General Organic Chemistry Sachin Kumar Ghose, New Central book agency.
20) Guidebook to Mechanism in Organic Chemistry by Peter Sykes, 6th Edition, Prentice Hall.
21) Advanced Organic Chemistry Part A: Structure and Mechanism and Part B:Reaction and synthesis ,Francis A. Carey, Richard J. Sundberg, 5th Edition, Springer .
22) Organic Chemistry Vol 1-2 I.L.Finar 5th edition,ELBS.

## M.Sc Semester – II (PRACTICALS)

## CHE411PR Organic Chemistry

Mixture analysis: ternary mixture to be given. (S+S+S )or ( L+L+L ). Type determination. Separation by physical and chemical methods. (both permitted in case of liquids)

## M.Sc Semester – II (PRACTICALS)

## CHE411PR 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 II
# CHE409 Physical Chemistry

**Unit I Statistical thermodynamics:**

Concepts of distribution of molecules, thermodynamic probability, permutations and combinations, Boltzmann's most probable distribution, partition function - translational, vibrational, rotational, electronic nuclear partition functions.

**Unit II Nuclear chemistry:**

Nuclear properties-nuclear radius, coulombic and nuclear potential radius, nuclear spin and angular momentum, magnetic moment, nuclear binding energy, nuclear models-shell model, liquid drop model, Fermi gas model, collective model, radioactive decay, nuclear reactions, evaporation, spallation, fragmentation, fission and fusion reactions, accelerators, reaction cross section, use of radioisotopes as tracers.

**Unit III Polymer chemistry:**

Kinetics and mechanism of polymer processes, criteria of polymer solubility, thermodynamics of polymer solutions, polymer characterization, molecular weight of polymer (number average and weight average) , methods of molecular weight determination, properties of polymers and applications.

**Unit IV Electrochemistry:**

Sign convention-American, European and IUPAC; Determination of dissociation constant of monobasic acids by conductometry, determination of dissociation constants of monobasic and polybasic acids by potentiometry.

The electrical double layer, the rate of charge transfer, polarization and overvoltage, basic principle of polarography, origin of different types of current; equation of polarographic wave, Ilkovic equation.

# M. Sc. Semester II- 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) Statistical thermodynamics – M.C.Gupta

(7) Polymer chemistry – Gowariker

(8) Polymer chemistry – Billmayer

(9) Principles of polymer science – Bahadur & Sastry

(10) Polymer science & technology – Fried

(11) Polymer chemistry- Malcolm P. Stevens

(12) Nuclear chemistry – Arniker

(13) Nuclear and radio chemistry – J.W. Kannedy, G.Friedlander

(14) Electrochemistry – Bockris and Reddy

# M.Sc. Semester II Practicals
# CHE412PR Physical Chemistry

**I. Conductometry**

1. Test of validity of Ostwald's dilution law and determination of dissociation constant of weak electrolyte like CH3COOH & ClCH2COOH
2. Verification of Debye-Huckel-Onsager's equation in case of strong electrolytes like HCl, KCl, NaCl.

**II Potentiometry**

1. Titration of dibasic acid like malonic, oxalic, succinic acid with NaOH and find the dissociation constant of acid.
2. Precipitation titration $\rightarrow$ Titration of halids with $AgNO_3$.
3. Redox titration Ferrous ammonium sulfate –$KMnO_4$ , $K_2Cr_2O_7$.

**III pH metry**

1. Determination of dissociation constant of weak acid like acetic and monochloroacetic acid

**IV Adsorption and kinetics**

1. Adsorption of acetic acid on activated charcoal
2. Determination of order of reaction between $K_2S_2O_8$ and KI by a fractional change method.

**V Distribution method**

1. Determination of the formula of the complex formed between cupric ion and ammonia by distribution method.

# M.Sc. Semester II- Practicals
# CHE412PR - Physical Chemistry

## 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 II
# CHE410 Analytical Chemistry

**UNIT-1**

**Sample Preparation Techniques**

Liquid-liquid extraction/solvent extraction-partition coefficient, distribution ratio and percent extraction. Solvent extraction of metal ions-ion association complexes and metal chelates, multiple batch extraction, Craig's counter-current distribution. Accelerated and Microwave assisted extraction, protein precipitation and solid phase extraction (SPE).

**UNIT-2**

**Chromatographic Methods**

Principles of chromatography, classification of chromatographic techniques based on mechanism of retention, configuration, mobile and stationary phase. Efficiency of separation- plate theory (theoretical plate concept) and rate theory (Van Deemter equation). Principles and applications of Paper chromatography, thin layer chromatography, HPTLC and Ion exchange chromatography. Counter-current chromatography for isolation of natural products.

**UNIT-3**

**pH metry and Conductometry**

pH measurement with glass electrode, working of glass electrode, mechanism of pH measurement, calibration of glass electrode, errors in pH measurement. Electrical conductance in solutions of electrolytes, measurement of conductance, conductometric titrations- acid-base, precipitation and complex formation titrations.

**UNIT-4**

**Potentiometry and Ion-selective electrodes**

Electrochemical cell, cell potentials, sign convention for electrode potentials, types of reference and indicator electrodes-metallic indicator and membrane indicator electrodes. Classification of membrane electrodes-ion-selective and molecular-selective electrodes. Principle, properties and design of ion-selective electrodes. Crystalline and non-crystalline membrane electrodes. Gas-sensing probes and enzyme substrate electrodes. Applications of potentiometric titrations**.**

# M.Sc. Semester II
# CHE410 Analytical Chemistry-Theory

**Reference Books**


1 "Quantitative Chemical Analysis" by Daniel C. Harris, 5th Edition, W.H. Freeman and Company, New York.

2 "Analytical Chemistry" by Gary D. Christian, 6th Edition, John Wiley and Sons Inc. New Jersey.

3 "Principles of Instrumental Analysis" by Douglas A. Skoog, 3rd Edition, Holt-Saunders International Editions.

## M.Sc. Semester II- Practicals
### Analytical Chemistry- CHE412PR

1. Determination of saponification value of oil.
2. Determination of iodine value of oil.
3. Determination of acid value of oil.
4. Determination of dissolved oxygen.
5. Determination of chemical oxygen demand.
6. Determination of iron in iron tablets.
7. Simultaneous estimation of chromium (III) and iron (III) by EDTA titration.
8. Simultaneous estimation of calcium (II) and zinc (II) by EDTA titration.
9. Simultaneous estimation of lead (II) and magnesium (II) by EDTA titration.
10. Separation of amino acids by TLC.
11. Separation of drugs by TLC.
12. Separation of dyes by TLC.

## M.Sc. Semester II- Practicals
### Analytical Chemistry- CHE412PR

# References

1. Analytical Chemistry Practice, John H. Kennedy, Saunders College Publishing, Second Edition 1990.
2. Vogels Textbook of Quantitative Chemical Analysis, $6^{th}$ Edition, 2002.