Inorganic Chemistry

Course Title: Inorganic Chemistry (Theory) **Credit:** Four (4) hrs.

Course No.: CHE-501 **Full Marks:** 100

Semester: First (1^{st}) **Pass Marks:** 50

Course Objectives:

- To provide a broad knowledge of the advanced inorganic chemistry and the principles of qualitative and quantitative analysis.

Course Contents:

Group A

Atomic Structure: Review lecture, Schrödinger wave equation, interpretation of the wave function, normalized and orthogonal wave functions, the principle of superposition, the particle in a one dimensional box, the particle in a three dimensional box, degeneracy, the hydrogen atom, transformation of coordinates, separation of variables, the Φ equation, the θ equation, spherical harmonics, the radial equation, quantum states, electron spin, energy states of the hydrogen atom, the self-consistent-field method, wave functions of the hydrogen atom, radial distribution curves, angular dependence of the wave function, atomic spectra and term symbols.

Group B

Covalent Bond: The variation method, ground state energy of hydrogen atom, the Secular equations, non crossing rule.

Hybridization: sp^3 hybridization, hybridization with d orbitals d^2sp^3 and dsp^2 hybridization, trigonal and diagonal hybrids, non equivalent hybrids, relative strength and angular distribution of hybrid orbitals, contours plots of hybrid orbitals, construction of hybrid orbitals, the effect of unshared pair on hybridization.

Group C

Molecular Orbital Theory: Molecular orbitals and its types, LCAO approximation, significance of resonance integral, hydrogen molecule ion (H_2^+), hydrogen molecule (H_2), other homonuclear diatomics, heteronuclear diatomics, experimental determination of molecular structure.

Valence Bond Theory: Valence bond method, hydrogen molecule (H_2), other homonuclear diatomics, heteronuclear diatomics, quantum mechanical structure and the meaning of resonance.

Group D

Analytical and Instrumental: A brief review on chemical analysis. Redox titration: use of potassium bromate, ceric salts, redox indicators, complexometric titration: metal ion indicators, adsorption titration: adsorption indicators, uses of common organic reagent in chemical analysis (dmg, oxine, cupferron).

Instrumentation, working principles and applications of following spectroscopic techniques: atomic absorption spectroscopy, atomic emission spectroscopy: flame photometry, atomic fluorescence spectroscopy, plasma emission spectroscopy (direct current plasma and inductively coupled plasma), molecular luminescence: fluorescence and phosphorescence, thermal analysis: thermo-gravimetric analysis (T.G.A), differential thermal analysis (D.T.A).

Reference Books for CHE-501:

1. F. A. Cottton and G. Wilkinson, *Advanced Inorganic Chemistry* (5th Edition) John Wiley and Sons Ins., 1988.
2. F. A. Cottton and G. Wilkinson and Paul L. Gauss, *Basic Inorganic Chemistry* (3rd Edition), John Wiley and Sons Incorporation, 1995.
3. J. E. Huheey, Ellen A. Keiter and Richard L. Keiter, *Inorganic Chemistry* (4th Edition), Harper Collins College Publishers, 1993.
4. J. Mendharm, R.C. Denny, J.D. Branes and M. Thomas, *Vogel's Textbook of Quantitative Chemical Analysis*, (6th Edition), 2008.
5. C. A Coulson, *Valence*, E.L.B.S., (2nd Edition), 1975.
6. M. C. Day and J. Selbin, *Theoretical Inorganic Chemistry*, East-west Press Pvt. Ltd., 1985.

7. G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, (5th Edition), 2014.
8. D. F. Shriver and P. W. Atkins, *Inorganic Chemistry*, (5th Edition) Oxford University Press.
9. D. A. Skoog, *Principle of Instrumental Analysis*, (3rd Edition), Saunders College Publishing, 1985.
10. H. H. Willard, L. L. Merritt, J. R. Dean and F. A. Settle, *Instrumental Methods of Analysis* (7th Edition), CBS Publishers and Distributions, India, 1986.
11. R. A. Day and A. L. Underwood, *Quantitative Analysis* (6th Edition), Prentice-Hall of India, 1993.
12. A. F. Wells, *Structural Inorganic Chemistry*, (4th Edition) Clarendon, Oxford, 1975.
13. P. J. Durrant and B. Durrant, *Introduction to Advanced Inorganic Chemistry*, Wiley (Interscience), (Latest Edition.), New York.
14. L. Pauling, *The Nature of the Chemical Bond* (Latest Edition), Cornell University Press.
15. R. McWeeny, *Coulson's Valence*, Oxford Press, 1979.
16. E. Cartmell and G.W. A. Fowles, *Valency and Molecular Structure* (4th Edition), Butterworth , 1997.
17. Bodie Douglas, Darl McDanniel and John Alexander, *Concepts and Models of Inorganic Chemistry*, (3rd Edition), John Wiley and Sons Inc., 1994.
18. G. H. Jeffery, J. Bassett, J. Mendharm and R. C. Denny, *Vogel's Textbook of Quantitative Chemical Analysis*,E.L.B.S., 1994.
19. F.A. Cotton, G. Wilkinson, C.A. Murillo and Manfred Bochmann , *Advanced Inorganic Chemistry*, (6th Edition), John Wiley and Sons, 1999.

Inorganic Chemistry

Course Title: Inorganic Chemistry Practical | **Credit:** Four (2) hrs.

Course No.: CHE-502 | **Full Marks:** 50

Semester: First (1^{st}) | **Pass Marks:** 25

Course Objective:

- To acquaint the students with quantitative and qualitative analytical methods.

Course contents:

Volumetric Analysis:

1. Determination of ferrous and ferric ions in a given mixture by potassium dichromate solution.
2. Determination of copper and iron in a given mixture by potassium dichromate solution.
3. Determination of percentage purity of pyrolusite by arsenious oxide.
4. Determination of copper as oxinate in the given copper sulphate solution by using potassium bromate.
5. Determination of percentage of "available chlorine" in bleaching powder by using potassium bromate.
6. Determination of zinc as oxinate in the given zinc sulphate solution by using potassium bromate.
7. Standardization of silver nitrate with the help of standard sodium chloride solution by Mohr's method.
8. Determination of amount of NaCl and KCl [and KCl and KBr] in a mixture by silver nitrate.
9. Determination of percentage purity of potassium bromide by using adsorption indicator.
10. Determination of amount of calcium, magnesium and manganese in a mixture by the use of EDTA.
11. Determination of hardness of water.

12. Determination of amount of copper and zinc in a mixture by EDTA.
13. Determination of total iron in a given sample of water.
14. Determination of ammonia in a given sample of water.

Any other experiments to be introduced in class work during the semester.

Reference Books for CHE-502:

1. M.R. Pokhrel, P.N. Yadav and S. Shrestha, *Advanced Practical Inorganic Chemistry* for M.Sc., (2^{nd} Edition), Kshitiz Publication, 2017.
2. A.I. Vogel, *Qualitative Analysis*; E.L.B.S., 1994.
3. Palmer, *Experimental Inorganic Chemistry*, Cambridge University Press, UK, 1954.
4. Angelici, *Synthesis and Technique in Inorganic Chemistry*; W.B. Sounders Co. (Sounders Golden Series), Philadelphia, 1991.
5. K. N. Ghimire, M. R. Pokhrel & K. P. Bohara, *University Experimental Inorganic Chemistry*, Quest Publication, Kirtipur, Kathmandu, 2008.

Physical Chemistry

Course Title: Physical Chemistry (Theory) **Credit:** Four (4) hrs.

Course No.: CHE-503 **Full Mark:** 100

Semester: First (1^{st}) **Pass Mark:** 50

Course Objectives:

- To introduce the basic concepts on advanced techniques for surface analysis of solids
- To provide knowledge on electro-analytical techniques, chemical kinetics & group theory

Course Contents:

Group A

Advanced Surface Characterization Techniques: Introduction of solid surfaces, *electron emission spectroscopic and imaging microscopic techniques*; *X-ray photoelectron spectroscopy (XPS)*: introduction, basic principle, instrumentation, XPS spectra, applications, advantages and limitations; basic principle, instrumentation, advantages and limitations of *Angle-resolved XPS* (ARXPS) and *Auger electron spectroscopy (AES)*:, comparison between XPS and AES; *scanning electron microscopy (SEM)*: introduction, basic principle, types of emitted electron for SEM, instrumentation, applications, advantages and limitations; *scanning probe microscopy (SPM)*: introduction, general principle of SPM, principle of scanning tunneling microscopy (STM), principle of atomic force microscopy (AFM), instrumentation of STM and AFM, different modes of STM and AFM, applications, advantages and limitations of SPM; *transmission electron microscopy (TEM)*: introduction, basic principle, modes, instrumentation, application advantages and limitations.

Group B

Electro-analytical Methods: Definition and classification of electro-analytical methods; basic principles of voltammetry; principal, instrumentation, applications and limitations

of DC polarography, pulse voltammetry (normal pulse, differential pulse, square wave), cyclic voltammetry, stripping voltammetry, AC voltammetry, amperometry (one electrode and two electrode system), Karl Fisher titration, coulometry, electrogravimetry and ion-selective electrodes (glass and solid state).

Group C

Chemical Kinetics: *Methods of fast reaction kinetics*: flow, relaxation, flash photolysis; *Polymerization kinetics*: derivation of rate equation for molecular and free radical mechanisms, cationic, anionic and emulsion polymerizations, related numericals; *Enzyme catalyzed reaction kinetics*: Michaelis-Menten mechanism of enzyme action, derivation of rate equation, graphical representations; influence of pH and temperature in enzyme action & related numericals; *Oscillating reaction kinetics*: introduction, Lotka-Volterra mechanism of chemical oscillation; *Diffusion controlled reactions in solution*: introduction, kinetics of diffusion-controlled reactions, kinetic salt effect, electron transfer reaction, potential energy surfaces; attractive and repulsive surfaces; classical trajectories: brief explanation with curve; related numericals.

Group D

Group Theory for Chemistry: Concept of Group Theory, group multiplication tables, cyclic and abelein groups, subgroups, similarity transforms, classes, symmetry elements, symmetry operations as group elements, consequences of symmetry, systematic classification of molecules into point group, matrix representations of symmetry operations and groups, reducible and irreducible representations, greater orthogonality theorem, character tables, properties of character tables and reduction formula, bond vectors and mathematical functions as bases for representations, basic concept of applications of group theory in chemical bonding and normal mode of molecular vibration (IR and Raman).

Reference Books for CHE-503:

1. C. R. Brundle, C. K. Evans, Jr., S. Wilson and L. E. Fitzpatrick (eds), *Encyclopedia of Materials Characterization: Surfaces, Interfaces, Thin Films,* Butxetworch-Heinemann, Reed Publishing (USA) Inc., 1992.
2. J. Bhattarai, *Frontiers of Surface Analysis*, (1st Edition), Balkhu, Kathmandu, Nepal.

2012.

3. C. D. Wagner, W. M. Riggs, L. E. Davis, J. F. Moulder and G. F. Mullenburge (eds), *Handbook of X-ray Photoelectron Spectroscopy*, Perkin-Elmer Co. Minnesota, USA, 1979.
4. J. Bhattarai, *Introduction to Electron Spectroscopy for In-depth Surface Analysis*, (1st Edition), Balkhu, Kathmandu, Nepal, 2011.
5. J. O'M. Bockris, A. K. N. Reddy and M. Gamboa-Aldeco, *Modern Electrochemistry, Fundamentals of Electrodics,* (2nd Edition), Vol. 2A, Kluwer Academic/Plenum Publishers, New York, 2000.
6. A. J. Bard and L. R. Faulkner, *Electrochemical Methods: Fundamentals and Applications,* (2nd Edition), John Wiley & Sons Inc., New York, 2001.
7. *Vogel's Textbook of Quantitative Inorganic Analysis*, (4th Edition), ELBS/Longman Scientific & Technical, London, 1978 (or more recent edition).
8. D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of Analytical Chemistry*, (8th Edition), International Student edition, Books/Cole Cengage Learning, Belmont, USA, 2004.
9. K. J. Laidler, *Chemical Kinetics*, Harper and Row, New York, 1988.
10. G. K. Vemulapalli, *Physical Chemistry*, Prentice-Hall of India Pvt. Ltd., New Delhi, 1997.
11. P. Atkins & J. de Paula, *Atkins' Physical Chemistry*, (10th Edition), Oxford University Press, New Delhi, 2014.
12. D. A. McQuarrie and J. D. Simon, *Physical Chemistry: a Molecular Approach*, Viva Student Edition, Viva Books Pvt. Ltd., New Delhi, 2011.
13. F. A. Cotton, *Chemical Applications of Group Theory*, (3rd Edition), John Wiley & Sons Inc., New York, 1990.
14. A. Salahuddin Kunju and G. Krishnan, *Group Theory and its Applications in Chemistry*, PHI learning Pvt. Ltd., New Delhi, 2010.

Physical Chemistry

Course Title: Physical Chemistry Practical | **Credit:** Two (2) hrs.

Course No.: CHE-504 | **Full Mark:** 50

Semester: First (1^{st}) | **Pass Mark:** 25

Course Objective:

- To make students capable of conducting physical chemistry experiments and analysis the data.

Course Contents:

Electrochemistry

1. Analyze the mixture of H_2SO_4, CH_3COOH and $CuSO_4$ with sodium hydroxide solution by conductometric method.
2. Determination of solubility product of sparingly soluble salt ($BaSO_4$) by conductometric method.
3. Potentiometric titration of a mixture of KCl and KI solutions and determine the concentration of KCl and KI solutions.
4. Preparation of standard buffer solution of CH_3COOH and CH_3COONa (pH 3.6, 4.0, 4.4, 4.8 & 5.2) and measure the solution pH using glass electrode and hence find out Nernstian slope.
5. Preparation of different buffer solutions using NH_4Cl and NH_4OH and measure the pH of solution by pH-meter using glass electrode and hence verify Henderson equation.

Chemical Kinetics

6. Energy of activation of acid catalyzed hydrolysis of methyl acetate.
7. Find the activation energy and the study the influence of ionic strength on the rate constant of reaction between $K_2S_4O_8$ and KI solutions.
8. Kinetics of the oxidation of iodide ions by H_2O_2 as an iodine clock reaction.

Miscellaneous

9. Calibration of common volumetric glass wares; pipette, burette and measuring cylinder.
10. Determine the enthalpy of neutralization of weak acid and strong base by using coffee cup calorimeter.
11. Determination of cross sectional area of –COOH group by measuring the variation of surface tension with concentration of butyric acid.
12. Plot current-voltage curves for given solutions of $CuSO_4$ and H_2SO_4 using platinum electrodes
13. Titration of iodine solution with sodium thiosulphate solution by the dead stop end point method or polarization method.

Any other experiments to be introduced in class work during the semester.

Reference Books for CHE-504:

1. J. N. Gurtu and A. Gurtu, *Advanced Physical Chemistry Experiments,* (6^{th} Edition), Pragati Prakashan, Meerut, India, 2014.
2. M. K. Sthapit and R. R. Pradhananga, *Experimental Physical Chemistry*, Taleju Prakashan, Kathmandu, 1998.
3. *Findlay's Practical Physical Chemistry*, (9^{th} Edition), revised by B. P. Levitt, Longman Group Ltd., London, 1973.
4. D. B. Khadka, *Practical Physical Chemistry*, Sunlight Publication (Student's Book), Kathmandu, 2009.

Organic Chemistry

Course Title: Organic Chemistry (Theory) **Credit:** Four (4) hrs.

Course No.: CHE-505 **Full marks:** 100

Semester: First (1^{st}) **Pass marks:** 50

Course Objectives:

- To provide the students basic knowledge about reaction mechanism.
- To familiarize important organic reagents used in synthesis.
- To acquaint the students with modern synthetic reactions.
- To provide the students basic knowledge of photochemistry.

Course Objectives:

Group A

Acids and Bases: Bronsted theory, the origin of acidity in organic compounds (factors influencing the acidity of an organic compounds), the mechanism of proton transfer reactions, acids and base solvents, measurement of solvent acidity (no mathematical derivation), acid and base catalysis (general and specific), Bronsted and Marcus equation, Lewis acids and bases, hard and soft acids and bases, the effects of structure on the strengths of acids and bases, effect of medium on acid and base strength.

Effects of Structure on Reactivity: Resonance and field effects, steric effects, quantitative treatments of the effect of structure on reactivity (The Hammett equation), substituent constant σ_x, reaction constant ρ, physical significance of σ_x, physical significance of ρ, uses of Hammett plots.

Group B

Aliphatic Nucleophilic Substitution: Review lecture (S_N1 and S_N2 reaction and mechanism with suitable examples, the neighboring-group mechanism, the neighboring–group participation by sigma and pi bonds, non-classical carbocations), ion-pairs in the SN1 mechanism, mixed SN1 and SN2 reactions, SET mechanism, nucleophilic

substitution at allylic carbon, nucleophilic substitution at vinylic carbon, nucleophilic substitution at a trigonal carbon, S_Ni reaction and mechanism.

Aromatic Nucleophilic Substitution: Introduction, S_NAr mechanism, the SN1 mechanism, $S_{RN}1$ mechanism, the benzyne mechanism.

Aromatic Electrophilic Substitution: Arenium ion mechanism, evidences for the arenium ion mechanism, the SE1 mechanism, orientation and reactivity in mono substituted benzene ring, ortho/para ratio, Ipso attack.

Aliphatic Electrophilic Substitution: Mechanisms, bimolecular mechanism S_E2 and S_Ei mechanism, S_E1 mechanism with suitable examples, electrophilic substitution accompanied by double bond shift.

Free Radical Substitution: Mechanisms, Free radical mechanism in general, free radical mechanism, mechanisms at an aromatic substrate, neighboring group assistance in free Radical Reactions, allylic halogenations.

Group C

Elimination Reaction: Review lecture, The E1 mechanism, E2 mechanism, E1cB mechanism, the E2C mechanism, the E1- E2- E1 CB spectrum, steric orientation of the double bond, reactivity– effect of substrate, structure, effect of attacking base, effect of leaving group, effect of the medium, mechanism and orientation in pyrolytic elimination, orientation of double bonds.

Synthetic Reactions and Reagents: Carbon-carbon bond forming reactions of organometallic reagents.

Carbon-carbon double bond forming reactions: Shapiro reaction, Bamford Steven reaction, Julia olefination reaction, Petersion chain olefination reaction.

Carbon-heteromultiple bond forming reactions: Passerini and Ugi reaction, Mannich reaction

Ring forming reactions: Pauson-Khand reaction, Demjenov cyclization.

Other synthetic reactions: Eschemoser-Tanabe ring cleavage reaction, Mitsunobu reaction, Stork enamine reaction, Michael reaction.

Group D

Photochemistry: Introduction, thermal and photochemical energy, activation energy, photochemical excitation, electronic transition, Jablonski diagrams, intersystem crossing,

photolytic cleavage, laws of photochemistry, quantum yield, photochemistry of carbonyl compounds, Norrish Type I and II-reactions, Paterno Buchii reaction, olefine photochemistry, photo dimerization, photoreduction of carbonyl compounds, photochemical oxidation, photo-rearrangement, photochemistry of α-, β-unsaturated ketones, photochemistry of aromatic compounds, introduction to electrocyclic reaction and cycloaddition.

Reference Books for CHE-505:

1. J. March, *Advanced Organic Chemistry*, (4th Edition), John Wiley and Sons, 1992.
2. Michael B. Smith, *March's Advanced Organic Chemistry*, (7th Edition), John Wiley and Sons, Inc., 2013.
3. Charles DePuy and Orville L. Chapman, *Molecular Reaction and Photochemistry*, *Prentice-Hall*, 1972.
4. I. L. Finar, *Organic Chemistry*, Vols. 1 and 2, ELBS, 1975.
5. Seyhan Ege, *Organic Chemistry Structure and Reactivity*, (3rd Edition), A.I.T.B.S. Publishers & Distributors, 1999.
6. Peter Sykes, *A Guide Book to Mechanism in Organic Chemistry*, (6th Edition), Pearson.
7. Education, Singapore, 1986.
8. R. Norman and J. M. Coxon, *Principles of Organic Synthesis*, CRC/CBS Publishers & Distributors, 1993.
9. I. Kumar, *Organometallic Compounds*, (5th Edition), Pragati Prakashan, Meerut, India, 2015.
10. J. Clayden, N. Greeves, and S. Warren, *Organic Chemistry*, (2nd Edition), Oxford University Press, India, 2014.

Organic Chemistry

Course Title: Organic Chemistry Practical | **Credit:** Two (2) hrs.

Course No.: CHE-506 | **Full Marks:** 50

Semester: First (1st) | **Pass Marks:** 25

Course Objective:

- To train the students in handing different equipments and train them further in identification, isolation and preparation of different compounds.

Course Contents:

1. Purification and drying of solvents and chemicals.
2. Experiments on chromatography.
3. An experiment on mixed melting point.
4. Identification of organic compounds containing mono and bifunctional groups such as aldehyde, ketone, carboxylic acid, ester, carbohydrate, phenol, hydrocarbon, amino group, nitro group, amide, ammonium salt etc and preparation of two derivatives for each.
5. Experiments on photochemistry.

Any other experiments to be introduced in class work during the semester.

Reference Books for CHE-506:

1. N. K. Vishnoi, *Advanced Practical Organic Chemistry* (3rd Edition), Vikas Publishing House Pvt. Ltd, 1996.
2. A. I. Vogel, *A Text Book of Practical Organic Chemistry* (5th Edition), Longman, 1989.
3. R. L. Shriner, R. C. Fuson and D. Y. Curtin and T. C. Morrill, *The Systematic Identification of Organic Compounds* (6th Edition), John Wiley & Sons, 1980.