SARDAR PATEL UNIVERSITY VALLABH VIDYANAGAR



SYLLABUS EFFECTIVE FROM: 2019-20 M. Sc. (Applied Chemistry) SEMESTER-I

PT01CACH21 Inorganic Chemistry – I

Unit – I Chemistry of Transition Elements – I

Concept of crystal field theory (CFT), ligand field theory (LFT) and molecular orbital theory (MOT), splitting of d-orbitals in various stereochemistry, Jahn Teller effect : tetragonal distortion in octahedral complexes; spectrochemical series, nephelauxetic series, Electronic states and term symbols; term symbols for diatomic molecule, microstates; derivation of terms for closed subshell; derivation of terms for p^2 and d^2 configurations.

Unit - II Chemistry of Transition Elements - II

Correlation diagrams; Orgel diagram; Tanabe-Sugano diagram; selection rule; determination of Dq and electronic parameters; Interpretation of electronic spectra of 3d metal complexes.

Unit –III Organometallic compounds

Introduction, classifications and general characteristics of organometallic compounds, Organometallic compounds of main group elements; Organometallic compounds of transition metals– σ -bonded and π -bonded organometallics, Catalytic processes involving transition metal organometallic compounds as homogeneous catalysts – hydrogenation, hydroformylation, oxidation, isomerization, dimerization and polymerization of alkenes and alkenes metathesis, Catalytic applications of main group organometallic compounds

Unit –IV Reaction Mechanism

The nature of substitution reaction, Theoretical approach to substitution mechanism, Nucleophilic reactivity, Nature of central atom, Kinetic application of crystal field theory, Replacement of coordinated metal, Acid analysis, Molecular rearrangement complexes, Reactions of geometrical and optical isomers, Outersphere electron transfer reactions, Innersphere electron transfer reactions, Two electron transfer.

Reference Books :

- Electronic Absorption Spectroscopy and Related Techniques, D. N. Sathyanarayana, University Press, 1st Ed. (2001).
- Advanced Inorganic Chemistry, Cotton, Wilkinson, Murillo and Bochmann, Wiley & Sons, 6th ed. (2007).
- Mechanism of Inorganic Reactions, F. Basolo, R. G. Persons, Wiley Pub. 2nd ed. (1967).
- Reaction Mechanism of Coordination Compounds, C. H. Langford, H. B. Gray (1966).
- Fundamental Principles of Inorganic Chemistry, D. Banerjea, Sultan Chand & Sons, 3rd ed. (1993).
- Organometallic Chemistry, R.C. Mehrotra, Anirudh Singh, New Age International (P) Limited Publishers, 2nd ed. (2000).

Books for further Reading :

- ▶ Introduction to Ligand Fields, B.N. Figgis, John Wiley & Sons, 1st ed. (1966).
- Modern Aspects of Inorganic Chemistry, Emeleus and Sharpe, Routledge & Kagan Paul Plc. 4th ed. (1973).
- Inorganic Chemistry, C. E. Housecroft, Alan G. Sharpe, Pearson Publication 4th ed. (2012).
- Inorganic Chemistry, James E. Huheey, Eilen A. Keiter, Richard L. Keiter, Harper Collins, Pearson Publication, 4th ed. (2006).
- ▶ Inorganic Chemistry, Shriver, Atkins, Oxford Press, 5th ed. (2009).
- Inorganic Chemistry, James E. huheey, Ellen A. Keiter, Richard L. Keiter, Pearson, 4th ed. (2006).
- Organometallic Compounds, Vol.1 & 2, G. E. Coates, M.L.H. Green, K. Wade, Metheun & Co. Ltd. London EC4, 3rd ed. (1967).
- ➢ Organometallic Compounds, G.E. Coates, John Wiley & Sons, Inc., 2nd ed. (1960).

PT01CACH22 Organic Chemistry – I

Unit – I Stereochemistry and Conformations :

Stereoisomerism, Concept of Chirality and molecular dissymmetry, Recognition of symmetry elements and chiral centers, Enantiomeric, Diastereomeric and Prochiral relationships. Conformations of acyclic molecules, Conformations of cyclohexane derivatives, Effect of conformation, angle strain, ring size, torsional and stereoelectronic effect on reactivity.

Unit - II Organic reactive intermediates & Aliphatic substitution reactions:

Organic reactive intermediates and mechanism: Types of organic reactions. Formation, structure, stability and reactivity of reactive intermediates, Factors influencing the reactivity of reactive intermediates. Electrophiles and nucleophiles.

Aliphatic substitution reactions: Nucleophilic Substitution reactions, Examples of nucleophilic substitution reactions, S_N^{1} , S_N^{2} and S_N^{i} reactions, their mechanism and stereochemistry. Effect of substrate's structure, nucleophile's nature, leaving groups and reaction medium on Nucleophilic Substitution reactions. Neighbouring Group Participation.

Unit - III Addition and elimination reactions:

Addition reactions, Mechanism and stereochemistry of the electrophilic, nucleophilic and free radical addition reactions, regio- and chemo-selectivity, orientation and reactivity. Examples of electrophilic addition on C=C bond and nucleophilic addition on C=X bonds (X=heteroatoms, like O and N).

Elimination Reactions, E1, E2 and E1cB mechanisms. Orientation in Elimination reactions. Hoffman versus Saytzeff elimination, Pyrolytic elimination reactions, Pyrolytic synelimination, competition between substitution and elimination reactions, Effects of substrate structures, attacking base, the leaving group, the nature of medium on elimination reactions. Addition-elimination reactions of carbonyl compounds.

Unit - IV Name reactions, rearrangements and their mechanism:

Rearrangement reactions: Bayer – Villiger, Beckmann, Fries, Hoffmann, Hoffmann-Martius, Lossen, Schmidt, Smiles, Sommelet-Hauser, Wittig, Wolff.

Name reactions: reactions involving enolates, condensation reactions, Mannich, Diels-Alder, Robinson annulation, Reimer-Tiemann, Simon-Smith, Ene Reaction, Barton, Hofmann-

Loffler-Freytag, Sharpless asymmetric epoxidation, Coupling reactions, Stark enamine, Cannizzaro Reaction, Ullmann, Vilsmeier-Haack.

Reference Books :

- Advanced Organic Chemistry, Part-A: Structure and Mechanisms, F.A. Carey, R. J. Sundberg, Kluwer Academic/ Plenum Publishers, Springer, 5th ed. (2008).
- Text book of Organic Chemistry Vol. I & II, I. L. Finar, Pearson Education India, 6th ed. (2002).
- ➤ Organic Chemistry, R. T. Morrison, R. N. Boyd, Pearson Pub., 7th ed. (2010).
- Advanced Organic Chemistry: Reaction Mechanism and Structure, Jerrry March, John Wiley, 4th ed. (2006).

Books for further reading :

- A Guidebook to Mechanism in Organic Chemistry, Peter Sykes, Pearson Pub., 6th ed. (2006).
- Organic Reaction Mechanism, R. K. Bansal, New Age International Pvt. Ltd. (2010), published in 2012.

PT01CACH23 Physical Chemistry – I

Unit – I Chemical Thermodynamics :

Introduction, revision of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Extensive and intensive properties, Gibbs-Duham equation and its application to study the partial molar quantities and their significance. Maxwell relations, thermodynamic equation of state, variation of chemical potential with temperature and pressure.

Unit – II Statistical Thermodynamics :

Limitation of classical thermodynamics, statistical thermodynamics, Energy states and energy levels, macrostate and microstate, thermodynamic probability, the Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac distributions, Molecular partition function and their significance, thermodynamics properties in terms of partition function, Rotational, translational, vibrational and electronic partition function, the statistical interpretation of entropy, Sackur-Tetrode equation, comparison of distribution function for indistiguishble particles.

Unit – III Phase Equilibria and Chemical Equilibria :

Elementary description of phase transitions, phase equilibria and phase rule, One-component, two components and three components system. Thermodynamics of ideal and non-ideal gases and solutions.

Unit – IV Electrochemistry :

Electrochemistry of solutions, Deye-Huckel theory of inter-ionic attraction, atmosphere, time of relaxation, relaxation and electro-phoretic effects, Dye-Huckel-Onsagar equation and its validity for dilute solution and at appreciable concentrated solutions. Activity coefficients : forms of activity coefficients and their interrelationship. Dye-Huckel limiting law for osmotic and activity coefficients of dilute electrolyte solutions and its application to concentrated solutions. Debye-Huckel-Bronsted equations, quantitative and qualitative verification of Dye-Huckel limiting law, Industrial applications of Electrochemistry.

Reference Books :

Thermodynamics for Chemists, S. Glasstone, D. Van Nostrand Publication, 13th print ed. (1964).

- Elements of Statistical Thermodynamics, L. K. Nash, Addison Wesley, 2nd ed. (1968).
- Elements of Statistical Thermodynamics, M. C. Gupta, New Age International Limited 2nd ed. (1990).
- Elements of Physical Chemistry, Peter Atkins, Julio De Paula, David Smith, Oxford University Press, 7th ed. (2017).
- Physical Chemistry, Ira N. Levine, Tata McGraw Hill Publishing House, 6th ed. (2011).
- Modern Electrochemistry Vol. I & II, J. O. M. Bockris, A. K. N. Reddy, Plenum Press, Springer publication, 2nd ed. (2018).
- An Introduction to Electrochemistry, S. Glasstone, Maurice Press, 1st ed. (2007).
- Electrolytic Solutions, R. A. Robinson, R. H. Strokes, Dover Publication, 2nd ed. Revised edition (2002).

Books for further reading :

- Thermodynamics of A Core Course, R. C. Srivastava, S. K. Saha, A. K. Jain, Prentice hall Learning Ltd. 3rd ed. (2007).
- An Introduction to Statistical Thermodynamics, T. L. Hill, Addison Wesley, 2nd Printing (1960).
- Statistical Mechanics, Donald A. McQuarrie, Viva student ed., (2011).
- An Introduction to thermodynamics, Kinetic theory of Gases and Statistical Mechanics, F. W. Sears and Slinger, Addition Wesley, 3rd ed. (1975).
- Principal of Physical Chemistry, B. R. Puri, L. R. Sharma, M. S. Pathania, V. P. D. Publisher, 47th ed. (2017).
- Elements of Physical Chemistry, S. Glasstone, MacMillan, 2nd ed. (1954).

PT01CACH24 Practicals

Inorganic Chemistry :

Quantitative Analysis:

Direct Titration (Cu⁺², Ni⁺², Ca⁺², Mg⁺² and Fe⁺³)

Indirect Titration of Calcium

By Back Titration and Replacement titration

Synthesis of metal complexes, double salts and estimation by gravimetry.

- $\blacktriangleright \quad \text{Chrome alum } K_2 SO_4, Cr_2 (SO_4)_3.24 \text{ H}_2 O$
- Ferrous ammonium sulphate FeSO₄(NH₄)₂SO₄.6H₂O
- Tris ethylene diamine Ni(II) sulphate
- ➢ Tetrammine Cu(II) sulphate
- Sodium trioxalato ferrate trihydrate
- > Potassium trioxalatochromate (III)
- ► Hexa-ammine nickel (II) chloride
- Hexa-ammine cobalt (III) chloride

Organic Chemistry :

- 1. Separation and identification of the two component mixtures using Chemical and physical methods.
- 2. Estimation of unsaturation, ester, acids, reducing sugars, phenols, amines, ketones.
- 3. Study on acid catalyzed synthesis reactions: Reaction of acetone with glycerol to synthesize acetal in presence of an acid catalyst
- 4. Study on base catalyzed synthesis reactions: Knoevenagel condensation of benzaldehyde with cyclohexanone

Reference Books :

- Qualitative Chemical semimicroanalysis, V. N. Alexeyev, Mir Publishers Moscow, 1st thus ed. (1975).
- ▶ Vogel's Qualitative Inorganic Analysis, G. Svehla, Orent Longman, 6th ed. (1979).
- Vogel's Textbook of Quantitative Chemical Analysis, G. H. Jeffery, J. Bassett, J. Mendham, R. C. Denney, ELBS Publication, 5th ed. (1996) Chapter 2, 3, 11.
- > A Textbook of Practical Organic Chemistry, A. I. Vogel, Longman, 5th ed. (2010).
- Elementary Practical Organic Chemistry Part 3: Quantitative Organic Analysis, A. I. Vogel, Longman, pearson edu., 2nd ed. (2010).
- Practical Organic Chemistry, F. G. Mann, B. C. Saunders, Longman. Pearson, 4th ed. (2009).

Laboratory Manual of Organic Chemistry, B. B. Dey, M.V.Sitaraman, Allied Publication, 1st ed. (1957).

PT01CACH25 Practicals

Physical and Analytical Chemistry :

- > Determination of normality, amount of chloride/bromide/iodide using Potentiometry.
- > Determination of solubility and solubility product of silver halides.
- Determination the composition of a mixture of acetic acid and Hydrochloric acid by Conductometric titration.
- > Determination of CMC of anionic surfactant by Conductometry.
- Determination of mixture of acids and relative strength of weak acids using Conductometry.
- > Investigate the molecular composition of a ferric-salicylate complex by Job's method.
- To determine the rate constant of the saponification of ethyl acetate at different temperatures and calculate the energy of activation of the reaction.
- To study the variation of refractive index with composition of mixtures of glycol and water.
- To find out the amount of Borax in given solution by titrating it against hydrochloric acid pH metrically.
- ▶ Kinetics of inversion of cane sugar in presence of strong acid.
- Investigation of the reaction between acetone and iodine.
- > Determination of partial molar volume by intercept method, density measurements.

Reference Books :

- Experiments in Physical Chemistry, J. M. Wilson, R. J. Newcombe, A. R. Denaro, R. M. W. Rickett, Pergamon Press, Oxford. (2nd revised and enlarged ed.) (2013)
- Findlay's Practical Physical Chemistry, B. P. Levitt, Longman Group Limited, 9th Edition.
- A Laboratory Manual of Experiments in Physical Chemistry, D. Brennan, C. F. H. Tipper, McGraw-Hill Publishing Company Ltd., London. 1st ed. (1967)
- Advanced Physico-Chemical Experiments: A Textbook of Practical Physical Chemistry and Calculations. J. Rose, Sir Isaac Pitman & Sons Ltd., London. 1st ed. (1964)
- Experimental Physical Chemistry, R. C. Das, B. Behera, Tata McGraw-Hill Publishing Company Ltd., New Delhi. 1st ed. (1983)

PT01EACH21 Analytical Chemistry

Unit - I Errors and Treatment of Analytical Chemistry :

Terms used in evaluation of Analytical data, Errors, Determinant, constant and interminate, Distribution of random errors, Average derivation and standard derivation, Variance and confidence limit, Significance figures and computation rules, Least square method., Methods of sampling : sample size, Techniques of sampling of gases, fluid, solids and particulates.

Unit - II UV-Visible and Infra-red (IR) Visible Spectroscopy :

Introduction of Spectroscopy, region of electromagnetic radiations, Interactions of radiation with matter, rotational, vibrational, electronic energy levels, types of spectroscopy methods. **UV-Vis :** Introduction, Beer-Lambert's law, instrumentation, fundamental of electronic transitions, chromophores and auxochromes, Woodward-Fieser rules, Effect of conjugation,

IR Spectroscopy : Introduction, Principle of IR spectroscopy, Instrumentation, fundamental modes of vibrations, types of vibrations, condition for IR absorption, selection rules, condition for IR absorption.

Unit – III Nuclear Magnetic Resonance (NMR) :

Introduction, principles, magnetic and nonmagnetic nuclei, precessional motion, Larmor frequency, absorption of radio frequency, instrumentation, Shielding and de-shielding effects, chemical shift, Origin of Chemical shift and spin-spin coupling, Fourier Transform technique, Pulse sequence, relaxation processes, peak area and proton ratio, anisotropic effect, spin-spin coupling, coupling constant, applications to simple structural problems, Nuclear Overhauser effect with examples.

Unit – IV Mass Spectroscopy :

General principle and theory, Methods of ionization, different detectors, time of flight, Importance of HRMS, Rules of fragmentation, Recognition of the molecular ion peak, Mclafferty rearrangements, metastable ionson peaks, the nitrogen rule, Application of Mass spectrometer in structure elucidation and molecular weight determination.

Reference Books :

Instrumental Methods of Analysis, Willard, Merrit, Dean and Settle, CBS Publishers & Distributors, 7th ed. (2004).

- Spectroscopic Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler, John Wiley & Sons, 2nd ed. (1967).
- Spectroscopic Methods in Organic Chemistry, D. H. Williams, I. Fleming, Tata McGraw Hills, 6th ed. (2004).
- Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West, Thomson Brookes/Cole, 9th ed. (2013).
- Introduction to Spectroscopy, Donald L. Pavia, Gary M. Lampman, George S. Kriz, Thomson Brooks/Cole publisher, 4th ed. (2009).
- Fundamentals of Molecular Spectroscopy, C. N. Banwell, E. M. McCash, Tata McGraw Hill publishing, 4th ed. (2017).

Books for further reading :

- Applications of Spectroscopic Techniques in Organic Chemistry, P. S. Kalsi, New Age Publication, 6th ed. (2014).
- Instrumental Methods of Chemical Analysis, V. K. Ahluwalia, ANE Books Publication, 1st ed. (2015).
- Spectroscopy, B. K. Sharma, GOEL Publishing House (2015).
- Atomic and Molecular Spectroscopy, Mool Chand Gupta, New Age International Publishers, 1st ed. (2001).
- Molecular Spectroscopy, J. D. Graybeal, McGraw Hill, Revised subsequent ed. (1993).
- Modern Spectroscopy, J. M. Hollas, John Wiley & Sons, 4th ed. (2003).

PT01EACH22 Environmental Chemistry

Unit – I Introduction to Environmental Chemistry

Introduction, Concepts and scope of study, useful terms, Environmental composition, nomenclature of some useful Terms, and ecology. Hydrosphere: Water resources, Physical and Chemical properties of water, sea water model, microbiological processes, organic and inorganic matters in water. Lithosphere: Concentric layers of earth, Physical and Chemical weathering processes, composition of soil, Nitrogen cycle and NPK in soil. Atmosphere: Composition & structure of atmosphere, particles, ions, radicals and chemical reactions in atmosphere. Biosphere: Definition, ecosystem and natural cycles

Unit – II Air and Water pollution

Air Pollution: Source and impact of air pollutants, classification of pollutants, environmental indicators. Sources and effect of air pollutants, pollution by SMOK, FOG, SMOG, PAN, PAH, greenhouse effect, acid rain, ozone depletion, EL Nino phenomena. Analysis of air pollution.

Water pollution: Definition, types of waters pollutants, Environmental toxicology and toxic elements & pesticides in water, Impact on enzymes, Biochemical effect of pesticides. Water and waste water analysis; collection of sample, Determinations of water quality parameters: Alkalinity, acidity, TDS, TH, D.O., BOD, COD, Chlorides, sulphate, nitrate and nitrite etc.

Unit - III Soil pollution and waste management :

Soil pollution and Waste management: Introduction to soil pollution; waste and pollutants in soil. Waste Management : Classification of wastes, overview of waste management program, methodologies, techniques available and new approaches, Green Chemistry : Basic Principle and its need, tools for green synthesis, Elementary ideas about Green process, green reagent, solvent, catalyst, atom economy.

Unit - IV Methods for Environmental Chemical Analysis :

Environmental chemical analysis methods Monitoring techniques in water and gas analysis: sampling, total solids, alkalinity and acidity, chlorides and sulfate, hardness, D.O., BOD, COD, nitrate and nitrite, analysis of pollutants in water, analysis of fuel gas, analysis of gaseous pollutants in air, Karl-Fisher reagent and its use, Instrumental techniques: atomic absorption spectrometry, X-ray fluorescence, gas chromatography etc.

Reference Books :

- Environmental Chemistry, J. W. Moore, E. A. Moore, Academic Press. Inc. Latest ed. (2012).
- Environmental Chemistry, A. K. De, New Age International Publishers, 7th ed. (2007).
- Principles of Environmental Science: Inquiry and Applications, William P. Cunningham, Mary A. Cunningham. McGraw Hill Publishing Company Ltd., 8th ed. (2016).
- Environmental Chemistry, S.K. Banerji, Prantice Hall of India Pvt. Ltd., 2nd ed. (2005).
- Handbook of Green Chemistry- Green Catalysis- Paul T. Anastas, Robert H. Crabtree, Wiley-VCH, 1st ed. (2013).
- Methods and Reagents for green synthesis: An introduction, Pietro Tundo, Alvise Perosa, F. Zecchin, Wiley, 1st ed. (2007).
- A Text Book on Experiments and Calculations-Engineering Chemistry, S. Chand & Co. Ltd. 1st ed. (1984).