CHEMISTRY

DSC-4: Inorganic and Physical Chemistry-II

Contact Hours: 56 **Work load: 4 Hours/Week.**

Credit Points :4

Evaluation: Continuous Internal Assesment-40 Marks

Semester End Examination -60 Marks

Course Objectives:

Students learn about

1. Different types of bonding in molecules/compounds/ions
2. The structures of molecules/compounds/ions based on different models/theories
3. Properties of compounds based on bonding and structure
4. The fundamentals of thermodynamics including the laws, the concept of entropy and free energy functions and their applications.
5. The concepts of surface chemistry, catalysis and their applications.
6. The theoretical and experimental aspects of chemical kinetics including basic theories of reaction rates and methods of determining order.
7. Electrochemistry dealing with electrolytes in solution. Conductance measurements and applications. Concept of ionic mobility and their determination.

Course outcomes: After the completion of this course, the student would be able to

1. Predict the nature of the bond formed between different elements
2. Identify the possible type of arrangements of ions in ionic compounds
3. Write Born - Haber cycle for different ionic compounds
4. Relate different energy parameters like, lattice energy, entropy, enthalpy and solvation energy in the dissolution of ionic solids
5. Explain covalent nature in ionic compounds
6. Write the M.O. energy diagrams for simple molecules
7. Differentiate bonding in metals from their compounds
8. Learn important laws of thermodynamics and their applications to various thermodynamic systems
9. Understand adsorption processes and their mechanisms and the function and purpose of a catalyst

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10. Apply adsorption as a versatile method for waste water purification.
11. Understand the concept of rate of a chemical reaction, integrated rate equations, energy of activation and determination of order of a reaction based on experimental data
12. Know different types of electrolytes, usefulness of conductance and ionic mobility measurements
13. Determine the transport numbers

Unit - I

Structure and Bonding -I

The ionic bond :Structures of ionic solids

Radius ratio rules, Calculation of some limiting radius ratio values, Coordination number 3 (planar triangle), Coordination number 4 (tetrahedral and square planar), Coordination number 6 (octahedral), Close packing. **3hrs**

Classification of ionic structures:

Ionic compounds of the type AX (ZnS, NaCl, CsCl)

Ionic compounds of the type AX_2 (Calcium fluoride (fluorite) and Rutile structure

Layer structures CdI_2 , Cadmium iodide structure

Limitations of radius ratio concept **2 hrs**

Lattice energy and Born-Haber cycle, Derivation of Born-Lande equation and its drawbacks, Kapustinskii equation, solvation energy and solubility of ionic solids, polarizing power and polarizability, Fajan's rules with applications.

Numerical problems **5 hrs**

Covalent bond: Valence bond theory, The Lewis theory,The octet rule, Exceptions to the octet rule, Sidgwick- Powell theory. Valence shell electron pair repulsion (VSEPR) theory, Effect of lone pairs, electronegativity, isoelectronic principle, Examples using VSEPR theory: BF_3 and BF_4^-, $NH_3$and NH_4^+, H_2O, PCl_5, ClF_3, SF_4, $I_3^-$and I_3^+, SF_6, and IF_7.

Limitations of VSEPR. **4 hrs**

Unit - II

Structure and Bonding -II

Concept of resonance, resonance energy, hybridisation, types of hybridization, sp, sp^2, sp^3 dsp^2 dsp^3, d^2sp^3, sp^3d^2 with one example each, and energetics of hybridization. Bent's rule, Limitations of Valence Bond Theory. **3 hrs**

Molecular Orbital theory:

LCAO concept: s-s, s-p, p-p, p-d and d-dcombinations of orbitals, bonding, nonbonding and antibonding molecular orbitals, non-bonding combinations of orbitals,Rules for linear combination of atomic orbitals

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Examples of molecular orbital treatment for homonuclear diatomic molecules H_2 molecule, H^+_2, He_2 molecule, He^+_2 molecule ion, Li_2 molecule, Be_2 molecule B_2 molecule, C_2 molecule, N_2 molecule, N_2^+, O_2 molecule, O_2^- and O_2^{2-}.
M.O. energy diagrams of heteronuclear diatomic molecules with examples (NO, NO^+ CO and HCl). Calculation of bond order, relationship between bond order, bond energy and bond length, magnetic properties based on MOT. **7 hrs**

Metallic Bonding:

General properties of metals : Conductivity, Lustre, Malleability and cohesive force
Crystal structures of metals and Bond lengths
Theories of bonding in metals:
Free electron theory, Valence bond theory, Molecular orbital or band theory of solids
Prediction of conducting properties of conductors. insulators and semiconductors, extrinsic and intrinsic semiconductors using M.O. theory. **4 hrs**

UNIT III

First Law of Thermodynamics

Thermodynamic Processes, Reversible and Irreversible Processes, Nature of Heat and Work, Internal Energy, First Law of Thermodynamics, Enthalpy of a System, Work done in isothermal and adiabatic expansion of an ideal gas, Numerical problems, Joule -Thomson Expansion, Relation between Joule-Thomson coefficient and other thermodynamic parameters.

Second law of Thermodynamics

Concept of entropy, thermodynamic scale of temperature, Statements of the Second Law of Thermodynamics, molecular and statistical interpretation of entropy, Calculation of entropy change for reversible and irreversible processes, Free Energy Functions: Gibbs and Helmholtz energy, Variation of S, G, A with T, V and P, Numerical problems, Free energy change and spontaneity, Gibbs-Helmholtz equation.

Third Lawof Thermodynamics

Statement of third law, concept of residual entropy, calculation of absolute entropy of molecules. **10 Hrs**

Surface Chemistry

Adsorption

Types of adsorption isotherms. Freundlich adsorption isotherm (only equation), its limitations. Langmuir adsorption isotherm (derivation to be done) and BET equation (derivation not included).

Catalysis

Types of Catalysis and theories with examples (intermediate compound theory and adsorption theory), Theory of acid base catalysis, Michaelis-Menten mechanism. Heterogeneous catalysis: surface reactions, unimolecular, bimolecular surface reactions. Autocatalysis with examples. Applications: Design process to removal of toxic compounds from industrial wastewater and treatment of portable water requirements.

4Hrs

UNIT IV

Chemical Kinetics

Differential and integrated form of rate expressions up to second order reactions, Derivation of expression of rate constant of second order reaction (a=b and a ≠ b), Problems on rate constant (a=b), Methods of determination of order of a reaction, temperature dependence of reaction rates; Arrhenius equation, activation energy, Numerical problems on Arrhenius equation in calculating energy of activation and rate constants. Collision theory of reaction rates, Lindemann's mechanism, qualitative treatment of the theory of absolute reaction rates. Experimental determination of kinetics of (i) inversion of cane sugar by polarimetric method (ii) spectrophotometric method for the reaction between potassium persulphate and potassium iodide. **7 Hrs**

Electrochemistry – I

Arrhenius theory of electrolytic dissociation. Merits and Demerits, Conductance, Specific conductance, equivalent and molar conductivity and their variation with dilution. Molar conductivity at infinite dilution. Numerical problems.

Kohlrausch's law of independent migration of ions and its applications, Debye-Hückel-Onsager equation. Ionic mobilities and their determinations, transference numbers and their relation to ionic mobility's, determination of transference numbers using Hittorf and Moving Boundary methods.

Applications of conductance measurement: (i) degree of dissociation of weak electrolytes (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts (iv) conductometric titrations (acid base titrations only) and (v) Hydrolysis constants of salts. Numerical problems. **7 Hrs**

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Reference Books

1. Peter Atkins & Julio De Paula, Physical Chemistry, 9th Ed., Oxford University Press (2010)
2. G W Castellan, Physical Chemistry, 4th Ed., Narosa (2004)
3. R G Mortimer, Physical Chemistry 3rd Ed., Elsevier: Noida, UP (2009)
4. B R Puri, L R Sharma and M S Pathania, Principal of Physical Chemistry, Vishal Publishing Co.
5. B S Bahl, G D Tuli and Arun Bahl, Essentials of Physical chemistry, S Chand & Company Ltd.
6. A S Negi and S C Anand, A textbook of Physical Chemistry, New Age International Publishers.
7. B N Bajpai, Advanced Physical chemistry, S Chand and Company ltd.
8. R L Madan, Chemistry for Degree Students, Semester I, II, III and IV, S Chand and Company Ltd.
9. P L Soni, O P Dharmarha and U N Dash, Textbook of Physical Chemistry, Sultan Chand and Sons.

PRACTICALS

Credit Points: 2 **Teaching Hours:4Hrs**

Evaluation : Continuous Internal Assessment-20 marks

Semester End Examination : 30 marks

Course objective:

To attain practical knowledge about:

1. Analytical skills in detecting the constituents present in unknown samples by systematically carrying out the qualitative analysis.
2. The methods of determining rates of chemical reactions.
3. Designing electrochemical cells and making measurements related to it.
4. Determination of physical characteristics of electrolytes using conductivity measurements in solution.
5. Adsorption phenomenon, mechanism and basic models to explain adsorption.
6. Simple techniques like conductometry to obtain physicochemical parameters of electrolytes.

Course outcomes: At the end of the course student would be able to

1. Understand the chemical reactions involved in the detection of cations and anions.
2. Explain basic principles involved in classification of ions into groups in semi-micro qualitative analysis of salt mixture
3. Carryout the separation of cations into groups and understandthe concept of common ion effect.

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4. Understand the choice of group reagents used in the analysis.
5. Analyse a simple inorganic salt mixture containing two anions and cations
6. Use instruments like conductivity meter to obtain various physicochemical parameters.
7. Apply the theory about chemical kinetics and determine the velocity constants of various reactions.
8. Learn about the reaction mechanisms.
9. Interpret the behaviour of interfaces, the phenomena of physisorption and chemisorptions and their applications in chemical and industrial processes.
10. Learn to fit experimental data with theoretical models and interpret the data

Part A- Inorganic Chemistry Practicals

Qualitative semi-micro analysis of mixtures containing 2 anions and 2 cations. Emphasis should be given to the understanding of different reactions.

The following cations and anions are suggested.

Cations: NH_4^+, Pb^{2+}, Bi^{3+}, Cu^{2+}, Al^{3+}, Fe^{3+}, Co^{2+}, Cr^{3+}, Ni^{2+}, Zn^{2+}, Mn^{2+}, Ba^{2+}, Ca^{2+}, Sr^{2+}, Mg^{2+}, Na^+, K^+ and Li^+.

Anions: CO_3^{2-}, CH_3COO^-, Cl^-, Br^-, I^-, NO_3^-, BO_3^{3-}, SO_4^{2-}, $C_2O_4^{2-}$ and PO_4^{3-}

Spot tests and flame tests to be carried out wherever possible.

Part B- Physical Chemistry Practicals

1. Determination of the enthalpy of neutralization of a strong acid with strong base.
2. Verification of Freundlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal.
3. The study of kinetics of potassium persulphate and potassium iodide volumetrically.
4. Determination of velocity constant for acid catalyzed hydrolysis of methyl acetate.
5. Determination of velocity constant for the saponification of ethyl acetate ($a = b$) volumetrically.
6. Determination of equivalent conductivity of strong electrolyte and verification of DHO equation.
7. Determination of dissociation constant of weak acid by conductivity method.
8. Conductometric titration of strong acid and strong base.
9. Conductometric titration of weak acid and strong base.
10. Determination of the hydrolysis constant of aniline hydrochloride conductometrically.
11. Determination of solubility product of sparingly soluble salt conductometrically.

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References

1. Vogel's Qualitative analysis, Revised by G. Svehla, Pearson education, 2002
2. J B Yadav, Advanced Physical Chemistry, Krishna Prakashan Media (P) Ltd, Meerut.
3. Khosla, B. D.; Garg, V. C. & Gulati, A. Senior Practical Physical Chemistry, R. Chand & Co.: New Delhi (2011).
4. Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. Experiments in Physical Chemistry 8th Ed.; McGraw-Hill: New York (2003).
5. Halpern, A. M. &McBane, G. C. Experimental Physical Chemistry 3rd Ed.; W.H. Freeman & Co.: New York (2003).

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Semester 4

B Sc / B Sc (Honors)

Title of the Course: **Open Elective: Electrochemistry, Corrosion and Metallurgy**

Number of Theory Credits	Number of lecture hours/semester
3	42

Evaluation Scheme for Theory:

Continuous Internal Assessment (CIA) – 40 Marks
Semester End Examination (SEE) – 60 marks

This course provides a broad introduction to the fundamental principles of Electrochemistry, Corrosion and Metallurgy. The student will gain an understanding of basic and practical applications in various fields of Electrochemistry, Corrosion and Metals and Alloy behaviour and manufacturing processes. This course is a valuable prerequisite for taking more technically challenging courses that will be required for career development.

Course Objectives

This course will deal with

1. Types of conductance, concept of electrolytes, electrolysis, redox reactions and EMF
2. Concept of different types of electrochemical cells, Types of electrodes and electrode potential. Application of electrochemical series.
3. Basic principles and applications of conductometric, potentiometric and pH titrations.
4. Different types of Batteries their principle construction and working - lead-acid storage and lithium ion battery. Study of Fuels cells.
5. Concept of corrosion, types of corrosion and its prevention by different methods. Introduction to electroplating.
6. Introduction to ores and minerals, extraction of metals from their ores, and purification. Eg., Manganese, Titanium and Uranium.
7. Study of alloys, classification, production and uses of alloys.

Expected Course Outcomes

Upon completion of the course students will be able to

1. Understand the concept of conductance in electrolytic solutions, electrolysis and redox reactions involved in electrode reactions.

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UNIT III

Metallurgy

Introduction: Ore, minerals, important ores of some common elements in India, General Principles of pyrometallurgy, roasting, Calcination, Gangue, Smelting, Flux, Gravity separation, Froth flotation process, leaching. Techniques employed for Purification of metal (Distillation process, Bessemerization, Electro-refining, Van Arkel and De Boer's Filament. 6 hrs

Extraction of metals: Extraction of Manganese (Pyrolusite), Titanium (Ilmanite) and Uranium. 4 hrs

Alloys: Introduction, Classification of alloys, commercially important alloys, gold karats, Production of Ferro alloys; Ferrochrome, Ferro Manganese, Uses of alloys. 4 hrs

Reference Books

1. Barrow. G.M, Physical Chemistry, Tata McGraw-Hill, (2007)
2. An introduction to electrochemistry, Samuel Glasstone, East-West edition New Delhi, (1942)
3. Text book of physical chemistry, Samuel Glasstone, 2nd Edition, Mac Millan India Ltd, (1991)
4. Principles and applications of Electrochemistry, D. R. Crow, 3rd edition, Chapmanhall London, (1988)
5. Fundamentals of electrochemical deposition, Milan Paunovic and Mordechay Schlesinger, Wiley Interscience Publications, New York, (1998)
6. Engineering Chemistry, V R Kulkarni and K Ramakrishna Reddy, New Age International, (2015)
7. Electrochemistry and Corrosion Science, Nestor Perez, Springer (india) Pvt. Ltd., (2004)
8. Principles and Prevention of Corrosion, D. A. Jones, Macmillan Publ. Co., (1996)
9. Essential of Materials Science and Engineering, Donald R. Askeland, Thomson Learning, 5th Edition, (2006)
10. Introduction to Engineering Materials, B. K. Agarwal, Tata McGraw Hill, 1st Edition
11. Material Science and Engineering, V. Raghavan, PHI Learning, 5th Edition
12. Engineering Materials and Metallurgy, R. K. Rajput, S. Chand - 1st Edition, (2011)

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