11.1.8. Course Code: DSC8: CHEMISTRY-3 (C3)
Course Title: CHEMICAL ENERGETICS AND EQUILIBRIA
Total Credits: 04 (Credits: Theory-02, Practical-02)
(Total Lectures: Theory- 30, Practical-60)

Objectives: The objective of this paper is to develop basic understanding of the chemical energetics, laws of thermodynamics and ionic equilibrium. It provides basic understanding of the behaviour of electrolytes and their solutions. The students will also learn about the properties of ideal and real gases and deviation from ideal behaviour.

Learning Outcomes:
By the end of this course, students will be able to:

- Understand the laws of thermodynamics, thermochemistry and equilibria.
- Understand concept of pH and its effect on the various physical and chemical properties of the compounds.
- Use the concepts learnt to predict feasibility of chemical reactions and to study the behaviour of reactions in equilibrium.

Unit 1: Chemical Energetics

Review of Intensive and extensive variables; state and path functions; isolated, closed and open systems, concept of heat, Q, work, W, internal energy, U, and enthalpy, H.

First law

Concept of heat, Q, work, W, internal energy, U, and statement of first law; enthalpy, H, relation between heat capacities, Joule Thompson Porous Plug experiment, Nature of Joule Thompson coefficient, calculations of Q, W, ΔU and ΔH for reversible, irreversible and free expansion of ideal gases under isothermal conditions.

Thermochemistry

Enthalpy of reactions: standard states; enthalpy of neutralization, enthalpy of hydration, enthalpy of formation and enthalpy of combustion and its applications, bond dissociation energy and bond enthalpy; effect of temperature (Kirchhoff's equations) on enthalpy of reactions.

Second Law

Concept of entropy; statement of the second law of thermodynamics. Calculation of entropy change for reversible processes and irreversible processes (for ideal gases). Free Energy Functions: Gibbs and Helmholtz energy; variation of S, G, A with T, V, P; Free energy change and spontaneity (for ideal gases), Gibbs-Helmholtz equation.

Third Law

Statement of third law, unattainability of absolute zero, calculation of absolute entropy of molecules, concept of residual entropy, calculation of absolute entropy of solid, liquid and gases.

(Lectures: 14)

Unit 2: Chemical Equilibrium

Criteria of thermodynamic equilibrium, chemical equilibrium in ideal gases. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient. Equilibrium constants and their qualitative dependence on T, P and concentration (Le Chatelier's principle). Free energy of mixing and spontaneity.

(Lectures: 04)

Unit 3: Ionic Equilibria

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, Ostwald's dilution law, ionization constant and ionic product of water, ionization of weak acids and bases, pH scale, common ion effect, salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions, Henderson-Hasselbach equation. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle.

(Lectures: 12)

PRACTICALS (Credits :02, Laboratory Periods: 60)

Chemical Energetics:

1. Determination of heat capacity of calorimeter.
2. Determination of enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
3. Determination of the enthalpy of ionization of ethanoic acid.
4. Determination of basicity of a dibasic acid by thermochemical method.
5. Determination of integral enthalpy of solution of salts (KNO_3 or NH_4Cl).
6. Determination of enthalpy of hydration of copper sulphate.

Ionic equilibria:

7. Preparation of buffer solutions: (i) Sodium acetate-acetic acid or (ii) Ammonium chloride-ammonium acetate. Measurement of the pH of buffer solutions and comparison of the values with theoretical values.
8. Study the effect of addition of HCl/NaOH on pH of the buffer solutions (acetic acid, and sodium acetate).
9. pH metric titration of (i) strong acid with strong base, (ii) weak acid with strong base

REFERENCES:

Theory:

- Castellan, G. W. (2004), Physical Chemistry, Narosa.
- Kapoor, K. L. (2015), A Textbook of Physical Chemistry, Vol 1, 6th Edition, McGraw Hill Education.
- Kapoor, K. L. (2015), A Textbook of Physical Chemistry, Vol 2, 6thEdition, McGraw Hill Education.
- Puri, B. R., Sharma, L. R. and Pathania M. S. (2020), Principles of Physical

Chemistry, Vishal Publishing Co.

Practical:

- Khosla, B. D.; Garg, V. C.; Gulati, A. (2015), Senior Practical Physical Chemistry, R. Chand & Co.
- Kapoor, K. L. (2019), A Textbook of Physical Chemistry, Vol 7, 1st Edition, McGraw Hill Education.
- Batra, S. K., Kapoor, V and Gulati, S. (2017) 1st Edition, Experiments in Physical Chemistry, Book Age series.

Additional Resources:

- Mahan, B. H.(2013), University Chemistry, Narosa.
- Barrow, G. M. (2006), Physical Chemistry, 5th Edition, McGraw Hill.

Teaching Learning Process:

- Conventional chalk and board teaching,
- Class interactions and discussions
- Power point presentation on important topics.

Assessment Methods:

- Class Tests at Periodic Intervals.
- Written assignment (s) / Presentation by individual students
- End semester University Theory and Practical Examination

Keywords: Chemical Thermodynamics, First law, Second law, Third law, Spontaneity of reaction, Equilibrium, buffers.