Course No: PGCHM17C203

Title: Physical Chemistry (04 Credits)

Max. Marks: 100 ***Duration****: 64 Contact hours*

Continuous Assessment: 20 Marks *End Term Exam: 80 Marks.*

Unit-I Quantum Chemistry **(16 Contact hours)**

General theory of angular momentum. Eigen functions and Eigen values of angular momentum operators. Ladder operators. Spin angular momentum, antisymmetry and Pauli's principle. Wave functions of poly-electron atoms, Slater determinant. Atomic term symbols, term separation of pn and dn configurations, spin-orbit coupling, Zeeman splitting.

Approximation methods: The Variation theorem, linear variation principle, application to hydrogen atom and helium atom. Perturbation theory: first order (non-degenerate & degenerate). Application of perturbation method to helium atom and anharmonic oscillator. Chemical Bonding: LCAO-MO approximation, H2+ molecular ion, brief introduction to H2. Molecular term symbols. Valence bond treatment of H2, comparison of MO and VB methods in the light of H2 molecule.

Unit-II Statistical Thermodynamics

(16 Contact hours)

Concept of distribution, thermodynamic probability and most probable distribution. Sterling approximation. Distribution Laws: Derivation of Boltzmann distribution law, Bose-Einstein and Fermi-Dirac laws (without derivation) and their comparison with Boltzmann distribution law.

Partition function: Significance, translational, rotational, vibrational and electronic partition functions. Calculation of thermodynamic properties in terms of partition functions, application to ideal monoatomic & diatomic gases. Equilibrium constant in terms of partition functions with application to isomerization and atomization reactions.

Unit-III Electrochemistry-I

(16 Contact hours)

ion-solvent interactions : Born model of ion-solvent interactions, Structural models of ion - solvent interations. Experimental determination of salt-solvent interactions.

Ion - ion interactions: Debye - Huckel theory of ion - ion interactions. Verification of Debye - Huckel limiting law. Activity, coefficients at moderate concentrations and higher concentrations. Activity coefficients as a function of ion-ion and ion-solvent interactions. Mean activity coefficients.

Debye-Huckel-Onsager conductance equation and brief idea of its extension. Metal-electrolyte electrified interface, concept of surface excess, thermodynamics of electrified interface, Lippman equation, electrocapillary curves. Methods for determination of surface excess.

Unit-IV Electrochemistry-II **(16 Contact hours)**

Structural models of metal-electrolyte interface: Helmholtz-Perrin, Gouy-Chapman and Stern models, recent advances. Semiconductor electrodes: Structure of semiconductor/ electrolyte interface

Theories of Heterogeneous Electron Transfer: Electron transfer at electrified interface at and away from equilibrium. Butller- Volmer equation, low and high field approximations, significance of transfer coefficient.

Books Recommended:

1. Physical Chemistry; P. W. Atkins: ELBS; Oxford; 1997.
2. Physical Chemistry- A Molecular Approach; D. A. McQuarie & J. D. Simon; University Science Books; 1997.
3. Introduction to Quantum chemistry; A. K. Chandra; Tata McGraw Hill; 1997.
4. Quantum Chemistry; Ira. N. Levine; Prentice Hall; 2000.
5. Quantum Chemistry; Prasad; New Age Publishers; 2000.
6. An Introduction to Statistical Thermodynamics; Robert P. H. Gasser and W. Graham Richards; World Scientific Publishing Co.; 1995.
7. Statistical Thermodynamics; M. C. Gupta; New Age International; 1993.
8. Statistical Mechanics; Agarwal, Eisner; Wiley; 1991.
9. Introduction to Statistical Thermodynamics; Chandler; OUP; 1987.
10. An introduction to Statistical Thermodynamics; Hill; Addison-Wesley; 1987.
11. An Introduction to Aqueous Electrolyte Solutions, Margaret Robson Wright, Wiley, 2007.

12. Modern Electrochemistry 1, 2A, 2nd Edition, J. O`M. Bokris and A. K. Reddy, Kluwer Academic/Plenum Publishers, New York.

13. Electrochemical methods, Fundamentals and Methods; A.J. Bard, L.R. Faulkner, Wiley; 1980.

14. Physical Electrochemistry- Fundamentals, Techniques and Applications; Eliezer Gileadi; Wiley-VCH; 2011.

15. Electrochemistry; 2nd Edition; Carl H. Hamann, Andrew Hammett, Wolf Vielstich; Wiley-VCH.

Teacher Incharge

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