Subject Code : P8CH13

CORE COURSE XIII - PHYSICAL CHEMISTRY II

UNIT – I

Quantum Chemistry – II & Group Theory

Applications of Wave mechanics, the rigid rotator, harmonic oscillator – Hydrogen atom solution – Shapes and nodal properties of orbitals – Space quantisation – electron spin – Many electron atoms – one electron orbitals – Pauli principle – derminental form of wave function, Helium atom and effective nuclear charge- Approximation methods – Variation methods, application to Hydrogen and Helium atoms– Perturbation method for nondegenerate systems.

Angular momentum in many electron systems – Spin orbit interaction, L-S and j-j coupling schemes.

Atomic Structure Calculation – Self consistent field method for atoms – Hartree and Hartree Fock method for atoms.

Vibrational spectra – symmetry properties of normal molecules – Symmetry co-ordinates – Selection rules for fundamental vibrational transition – IR and Raman activity of fundamentals in CO2, H2O, N2F2 – The rule of mutual exclusion and fermi resonance.

UNIT - II
Electrochemistry - I

Electrolytic conductance Debye-Huckel-Onsager theory – Debye Falkenhagen and Wien effect. Electrode – electrolyte equilibrium, electrode potential – concentration cells – liquid junction potentials.

Processes at Electrodes- The rate of charge transfer - current density – Butler – Volmer Equation – Tafel equation – Electrical double layer potential – Theory of multiple layers at electrode – electrolyte interfaces – Double layer capacity – Electrokinetic phenomena, Applications: Fuel cells and power storage.

UNIT – III
Electrochemistry - II

Principles and applications of polarography – Instrumentation, Types of cells, advantages of dropping mercury electrode, interpretation of current voltage curves, tests for reversibility, determination of 'n' values (usefulness of Illkovic equation), polarographic maxima, current time curves, Modern developments, Oscillographic polarography, AC polarography – Cyclic Voltammetry, advantages over polarographic techniques – test of reversibility of electron transfer reactions – Chronopotentiometry – apparatus used, advantages over polarography – controlled potential coulometry.

UNIT - IV
Surface Phenomena and Kinetics:

Surface Phenomena: Gibbs adsorption isotherm – solid- liquid interfaces – contact angle and wetting – solid-gas interface – physisorption and chemisorption – Langmuir, BET isotherms – surface area determination. Kinetics of surface reactions involving adsorbed species – Langmuir-Hinshelwood mechanism, Langmuir – Rideal mechanism – Rideal –Eley mechanism. Some interfacial aspects on Micelles, Reverse micelles, Micro emulsions and Membranes.

Chemical Kinetics-II

Application of ARRT to solution kinetics - Effect of solvent and ionic strength, influence of pressure on rates in solution - Enzyme catalysis- Mechanism of single substrate reactions – Michaelis Menton law – Kinetics of processes in micellar and reverse micellar systems.

UNIT – V

Molecular Thermodynamics-II

Third law-thermodynamics-Need for it-Nernst heat theorem and other forms of stating the third law. Thermodynamic quantities at absolute zero – Apparent exceptions to the third law.

Thermodynamics of systems of variable composition – partial molar properties – chemical potential – relationship between partial molar quantities – Gibbs Duhem equation and its applications (the experimental determination of partial molar properties not included).

Thermodynamic properties of real gases – fugacity concept – calculation of fugacity of real gas – Activity and activity coefficient – concept – definition – standard states and experimental determinations of activity and activity coefficient of electrolytes.

References

Text Book

1. F.A. Cotton, Chemical Applications of group Theory, 2nd ed., Wiley Eastern 1971
2. A.K. Chandra, Introductory Quantum Chemistry, 4th ed., Tata McGraw Hill, 1994
3. D.A. Mcquarrie, Quantum Chemistry, University Science Books, 1983.
4. J.P. Lowe, Quantum Chemistry, Academic Press, 1978.
5. I.N. Levine, Quantum Chemistry, Allyn and Bacon, 1983.
6. P.W. Atkins, Physical Chemistry, ELBS and Oxford University Press, Oxford, 1983.
7. S.Glasstone, Introduction to Electrochemistry, Affiliated East-West Press, 1968.
8. J.Albery, Electrode Kinetics, Clarendon Press, Oxford Chemical Series, 1979.
9. D.R.Crow, Polarography of Metal Complexes, Academic Press, New York.
10. Daniel C Harris, Quantitative Chemical Analysis, 4th ed., W. H. Freeman and Company, New York, 1995
11. J. Rajaram and J.C.Kuriacose, Thermodynamics for Students of Chemistry – Classical, Statistical and Irreversible, Shobhan Lal Nagin, New Delhi, 1981.
12. G.W.Castellan, Physical Chemistry, Narosa, New Delhi, 1986.
13. I. M. Klotz and P.M.Rosenberg, Chemical Thermodynamics: Basic Theory and Methods, 3 edn. W.A. Benjamin, New York, 1974.
14. K.J. Laidler, Chemical Kinetics, 2nd ed., Tata McGraw Hill, 1975.
15. A.A. Frost and R.G. Perason, Kinetics and Mechanisms, John Wiley & Sons, New York, 1953.
16. I.Amdur and G.G. Hammes, Chemical Kinetics Principles and Selected Topics, McGraw Hill, New York, 1966.
17. M. Gratzel and K. Kalyanasundaram, Kinetics & Catalysis in Microheterogeneous Systems, Academic Press, New York, 1991.
18. J.I. Steinfeld, J.S.Francisco and W.L. Hase, Chemical Kinetics and Dynamics, 2nd edn, Prentice Hall, New Jersey, 1999.
19. R.K.Dave, Chemical Kinetics, Campus Books, 2000.