

Course Code	Course Title	C	H	I	E	T
17P1CMC3	PHYSICAL CHEMISTRY-I	4	4	25	75	100

UNIT I PROPERTIES OF GASES AND LIQUIDS 12 Hrs

Equations of states-Molecular speeds-Max Well distribution of molecular velocities- one, two and three dimensions-Energy distribution-Maxwell-Boltzmann distribution law-Principle of equipartition of energy and heat capacity-Rotation, vibration and Translational degree of freedom-Molecular collisions-Mean free path-Transport properties-Thermal conductivity-Viscosity and diffusion of gases.

Liquid State-Theory of liquids-Internal Pressure-Liquid crystals-Nematic, Cholesteric, Smectic-Theory and application in liquid crystal display.

UNIT II THERMODYNAMICS 12 Hrs

Thermodynamic equations of state - derivation and application to real gases in the calculations of $(dH/dp)_T, (dE/dv)_T$ and $\mu_{J,T}$ etc. Thermodynamics systems of variable composition. Partial molar properties : Chemical potential: Definition - Gibbs-Duhem equation. Determination by graphical method. Variation of chemical potential with temperature and pressure. Fugacity: Definition - Determination of fugacity. Variation of fugacity with temperature and pressure. Activity: Definition –Determination of activity and activity coefficient of non-electrolytes by vapour pressure measurements. Dependence of activity on temperature and pressure. Third law of thermodynamics: absolute entropies – determination of absolute entropies – exceptions to third law.

UNIT III QUANTUM CHEMISTRY- I 12 Hrs

Black Body radiation –de Broglies wave particle duality- Experimental verification of matter waves-Compton effect-Heisenberg's Unvertinity principle-The schrodinger wave equation, Postulates of Quantum mechanics, Operators – Linear operator, commuting operators, Hermitian operator. Eigen functions and Eigen values, Orthogonality and Normalisation. Discussion of solutions of Schrödinger equation to particle in a One Dimensional Box, Three Dimensional Box, The Simple Harmonic Oscillator, The Rigid rotator, The H- atom, Probability Distribution curves, Angular momentum Eigen functions and Eigen Values of angular momentum.

UNIT IV QUANTUM CHEMISTRY- II 12 Hrs

Approximation methods – The Variation theorem, Linear variation principle, Application of variation method to He – atom, Perturbation theory (only Time independent, First order and non-degenerate), Application of Perturbation Theory to He-atom. Hartree Fock Self consistent Field Theory, Symmetric and Antisymmetric Wave functions, Pauli's exclusion principle of

Antisymmetric wave functions, Huckel Molecular orbital theory – Huckel theory of conjugated system-Delocalization Energy, Bond order and Charge density Application of HMO to ethylene, butadiene and cyclopropenyl system.

UNIT V CHEMICAL EQUILIBRIUM AND PHASE RULE

12 Hrs

Chemical equilibrium: Thermodynamic derivation of equilibrium constant (K_p) for equilibrium involving ideal gases and real gases – van't Hoff reaction isotherm. Heterogeneous equilibrium: Definition – examples - Le Chatelier and Braun Principle - thermodynamic proof - temperature, pressure and concentration dependence. Van't Hoff equation: Derivation and applications. Simultaneous equilibria: Free energy and equilibrium constant.

Basic terminologies of phase rule: - Three component system: three liquid system, one liquid and two solid systems and two liquid and one solid system – three solids system.

Text Book(s):

1. Glasstone, S., “Thermodynamics for Chemists”, First Edition, van Nostrand & Co., New York, 2005.
2. Rajaram, R. and Kuriacose, J.C., “Thermodynamics”, Second Edition, S. Chand and Co., New Delhi, 1993.
3. Kapoor, K.L., “A Text Book of Physical Chemistry”, Volumes 2 & 5, Fourth Edition, Macmillan India Ltd., New Delhi, 2011.
4. Mc Quarrie, D.A. and Simon, J.D., “Physical Chemistry- A Molecular Approach”, First South Asian Edition, Viva Books Pvt. Ltd., New Delhi, 2011.
5. Chandra, A.K., “Introductory Quantum Chemistry”, Fourth Edition, Tata-McGraw Hill Publication Co. Ltd., New Delhi, 2010.
6. Atkins, P. and de Paula, J., “Physical Chemistry”, Ninth Edition, Oxford University Press, New Delhi, 2011.
7. Ball, D. W., “Physical Chemistry”, First Indian Edition, Cengage Rearing India Pvt., Ltd., New Delhi, 2009.

Reference Books:

1. Mortimer, R.G., “Physical Chemistry”, Third Edition, Academic Press – An imprint of Elsevier, London, 2009.
2. Engel T. and Reid, P. “Physical Chemistry”, Second South Asian Edition, Pearson Publication, New Delhi, 2011.
3. Berry, R.S., Rice, S.A and Ross. J, “Physical Chemistry”, Second Edition, Oxford University Press, New York, 2007.
4. Puri, B.R., Sharma, L.R. and Pathania, M.S., “Principles of Physical Chemistry”, Forty Sixth Edition, Vishal Publishing Co., Jalandhar, 2013.
5. Bhal, A., Bhal, B.S. and Tuli, G.D., “Essentials of Physical Chemistry”, First Edition, S. Chand & Company Ltd., New Delhi, 2012.