PHYSICAL CHEMISTRY (BS-ADP 5th Semester)

Module Code:	**Chem-302**
Module title:	**Quantum Chemistry**
Name of Scheme:	**BS-ADP 5th Semester**
Department:	**School of Chemistry**
Faculty:	**Science**
Module Type:	**Compulsory**
Module Rating:	**2 credits**

OBJECTIVES

This course will help in understanding basic principles of kinetic theory of gases and quantum chemistry. This will assist students in calculating bond energies and bond length on the basis of quantum approach.

SYLLABUS OUTLINES

Postulates of quantum theory, Eigen functions, operators, Schrödinger's wave equation, particle in one dimensional box, Normalized wave function and orthogonality, Quantum mechanical tunneling, motion of particle in three dimensional box and idea of degeneracy, separation of variables and derivation of quantum numbers, Mathematical treatment of rigid rotator and calculation of bond length of simple molecules, harmonic oscillator and calculation of bond length of simple molecules, harmonic oscillator and calculation of vibrational frequencies, formation of covalent bond, Mathematical treatment of He_2+ and H_2 molecules, discussion of overlapping integrals, molecular orbital theory and formation of H_2 and O_2 molecules. The van der walls equation, Maxwell distribution of molecular velocities and energies, Derivation of average velocity and most probable velocity, Barometric formula, Maxwell-Boltzmann's law of energy distribution

RECOMMENDED BOOKS

1. Bhatti, H. N. and Farooqi, Z. H., Modern Physical Chemistry, Revised ed., Caravan Book House, (2014).
2. Physical Chemistry, Samuel Glasstone, 1995. Macmillan and Co. Ltd. St. marlins Street, London.
3. Principles of Physical chemistry, Maron and Prutton, 1965 the Macmillan Company, Collier Macmillan Ltd. London.
4. Physical Chemistry, Barrow, 1973, McGraw Hill, Tokyo.
5. Physical Chemistry, Moore, 1972, Rentice Hall, Englewood cliffs, Jersey.
6. Physical Chemistry, Alberty and Daniels, 1962, McGraw Hill Book Company Ltd London.
7. Physical chemistry, Atkins, 1989, Oxford University Press, Walton Street, Oxford.
8. Physical Chemistry, Castallan, 1972, Addson Westey Publishing Company, Menla Park, California, London.