



## Quantum Chemistry

Course Code	Course Num.	Course Name	Credit Hours	Lec	Lab	Tut	Prerequisites
CHM	345	Quantum Chemistry	2	2	0	0	CHM 242

### Objectives:

- Improve the students' knowledge of the principles of quantum theory.
- Use the techniques and applications, atomic structure, Wave functions, operators, observable, eigen values, and eigene functions.
- Describe the translational motion of particle in 1-D box.
- Give a brief summary about the electronic transitions (Fluorescence and Phosphorescence, and laser action).

### Syllabus:

Classical Mechanics, Rotational motion, Harmonic Oscillator. Equipartition theorem, Black-Body radiation, Planck Distribution. Photo electric effect, Atomic and Molecular spectra. Wave functions, operators, observable, Eigen values, and Eigen functions, Schrodinger Equation . Normalization of wave function, Quantization. Balancing.

Translational motion, Particle in a box. Motion in two dimensions, Degeneracy, Vibration motion (harmonic motion). Rotational motion in two dimensions, Quantization of rotation. Rotation in three dimensions, Spin quantum numbers.

Structure and spectra of Hydrogen atoms. Atomic orbitals and Shells and sub shells. Spectral transitions and selective rules, Structures of many electron atoms, orbital approximation (electronic structure by configuration in ground state). Spin - orbit coupling. Term symbols and selective rules. Multiplicity. Total angular momentum. Russell-Saunders coupling Scheme.

Rotational spectroscopy. Rotational energy levels. spherical, symmetric, and linear rotors. Degeneracies and the Stark effect. Rotational transitions . Vibrations of diatomic molecules. Vibration- Rotation spectra. Electronic Transitions, Franck-Condon principle, Fluorescence and phosphorescence, and Laser action.

### Textbooks:

Atkins, P., and J. de Paula. Physical Chemistry. 8th ed. New York, NY: W.H. Freeman and Company, 2001 ( ISBN: 9780716735397)

### References:

1. K. J. Laidler, J. H. Meiser, B. C. Sanctuary, Physical Chemistry, Houghton Mifflin Company, 2003, 4th Ed or later
2. G.M. Barrow "Physical Chemistry" 5th Edition, McGraw-Hill
3. Ira N. Levine "Physical Chemistry" 5th Edition, McGraw-Hill ( ISBN: 0-07-231808-2)
4. Silbey, R., R. Alberty, and M. Bawendi. Physical Chemistry. 4th ed. New York, NY: John Wiley & Sons, 2004. ISBN: 9780471215042

