PHY-917 Atomic and Molecular Spectroscopy

Credit Hours: 3-0

Prerequisite: None

Course Objectives: The overall goal of this course is to establish how basic concepts of quantum mechanics can be utilized to quantitatively explain atomic and molecular spectra. This course will help students understand that spectroscopic data cannot be understood without quantum mechanics.

Core Contents: The electromagnetic field and its interaction with charged particles, transition rates and dipole approximation, the Lamb shift , hyperfine structure and isotopes shift, the independent particle model, the Hartree Fock approximation and the self-consistent field, general nature of molecular structure, the structure of polyatomic molecules, rotational energy levels of diatomic molecules, laser and basics of optical spectroscopy, nuclear magnetic resonance spectroscopy and ion cyclotron resonance mass spectrometry

Detailed Course Contents: The electromagnetic field and its interaction with charged particles, The electromagnetic field and its interaction with charged particles, The transition rates and dipole approximation, Deriving selection rules for one electron atoms, Photoelectric effect, The Lamb Shift , Hyperfine structure and isotopes shift, The Schrödinger Equation for two electron atoms, Spin wave functions and role of Pauli Exclusion Principle, The independent particle model, The ground-state of two electron atoms, Excited states of two electron atoms, Central Field approximation for many electron atoms, The Hartree Fock approximation and the self-consistent field, General nature of molecular structure, The Born-Oppenheimer separation of Diatomic molecules, The rotation and vibration of diatomic molecules, Electronic structure of diatomic molecules, The structure of polyatomic molecules, Rotational energy levels of diatomic molecules, Vibrational spectra of diatomic molecules, Electronic spectra of diatomic molecules, Laser: Physical principles, Optical resonator, Single mode laser, Types of laser, Nonlinear optics, Generation of short laser pulse, Basics of Optical Spectroscopy: Absorption of light, Infrared and

Raman spectroscopy, UV/VIS absorption and Luminescence, Nuclear magnetic resonance spectroscopy: Nuclear magnetic moment in a magnetic field, Principle of NMR spectroscopy, Application of NMR spectroscopy, Ion cyclotron resonance mass spectrometry: Conventional mass spectrometry, ICR mass spectrometry, Fourier transform in ICR mass spectrometry.

Course Outcomes: On successful completion of this course, students will be able to

- derive the energy shifts due to corrections using first order perturbation theory
- understand the state and explain the key properties of many electron atoms and the
  importance of the Pauli exclusion principle
- understand the contributions of transitions between rotational, vibrational and electronic
  states to the spectra of diatomic molecules, vibrations and electronic structure of polyatomic molecules.
- Understand the basic spectroscopic techniques (Optical Spectroscopy, Nuclear magnetic
  resonance spectroscopy and Ion cyclotron resonance mass spectrometry)

Textbooks:

1. B. H. Bransden and C. J. Joachain, Physics of Atoms and Molecules, 7th ed. McGraw Hill 2006. (Referred as BJ)
2. Wolfgang Demtröder, An Introduction to Atomic and Molecular Physics, 6th ed. McGraw-Hill 2003. (Referred as WD)
3. G. Gauglitz and T. Vo-Dinh, Handbook of Spectroscopy, Wiley-VCH 2003. (Referred as GT)
4. Jyrki Kauppinen, Fourier transforms in spectroscopy, Wiley-VCH, 2005. (Referred as JK)

Reference Books:

Peter Hannaford, Femtosecond Laser Spectroscopy, Springer Science & Business Media, Inc., 2005.

Weekly Breakdown		
Week	***Section***	***Topics***
1	BJ 4.1	The electromagnetic field and its interaction with charged particles
2	BJ 4.1-4.3	The electromagnetic field and its interaction with charged particles, The transition rates and dipole approximation
3	BJ 4.5,4.8	Deriving selection rules for one electron atoms, Photoelectric effect.
4	BJ 5.4-5.5	The Lamb Shift, Hyperfine structure and isotopes shift
5	BJ 6.1-6.3	The Schrödinger Equation for two electron atoms, Spin wave functions and role of Pauli Exclusion Principle.
6	BJ 6.4-6.6	The independent particle model, The ground-state of two electron atoms, Excited states of two electron atoms.
7	BJ 7.1	Central Field approximation for many electron atoms
8	BJ 7.4	The Hartree Fock approximation and the self-consistent field.
9	BJ 9.1-9.3	General nature of molecular structure, The Born-Oppenheimer separation of Diatomic molecules, The rotation and vibration of diatomic molecules
10	BJ 9.4-9.5	Electronic structure of diatomic molecules, The structure of polyatomic molecules
11	BJ 10.1-10.3	Rotational energy levels of diatomic molecules, Vibrational spectra of diatomic molecules, electronic spectra of diatomic molecules
12	WD 8.1-8.6	Laser: Physical principles, Optical resonator, Single mode laser, Types of laser, Nonlinear optics, Generation of short laser pulse.
13	GT 3.1-3.4	Basics of Optical Spectroscopy: Absorption of light, Infrared and Raman spectroscopy, UV/VIS absorption and

		Luminescence
14	JK 7.1, 7.2, 7.3	Nuclear magnetic resonance spectroscopy: Nuclear magnetic moment in a magnetic field, Principle of NMR spectroscopy, Application of NMR spectroscopy
15	JK 8.1-8.3	Ion cyclotron resonance mass spectrometry: Conventional mass spectrometry, ICR mass spectrometry, Fourier transform in ICR mass spectrometry