C10J ATOMIC STRUCTURE (6 lectures)

Introduction

The Atomic Structure course is considered as an important part of the core course for Introductory Chemistry as concepts which are learnt here will be employed in the subsequent sections on Physical, Inorganic (e.g. bonding and antibonding orbitals) and Organic Chemistry (e.g. hybridization). This covers basic and fundamental principles which are common to all areas of Chemistry. You are encouraged at this early stage in the degree programme, not to form, or create, an imaginary boundary which separates the different disciplines of Chemistry, but to search for and make the links which will make understanding the different topics more enjoyable.

Atomic structure refers to the configuration of the constituents of the atom. When we speak of electronic configuration we deal with information that tells us where in the atom the electron(s) is (are) found. The chemistry of an element is determined largely by its electronic configuration, so it is very important to get as much information as possible about the behaviour of electrons in atoms.

It is a good idea to start with the simplest atom, which is Hydrogen, and try to find out as much as possible about it. Here we refer to the isotope with 1 proton and 1 electron. Do we know everything about the electron in the hydrogen atom? Do we really understand what is meant by the phrase "The electron in the ground state hydrogen atom resides in the **1s** orbital?" Do we know where the electron is in the hydrogen atom? How does it move about in the atom? These are some of the questions which we will try to address in this section. After we have gained information about the behaviour of the electron in the ground and excited states of the hydrogen atom, then we will try to apply what we have learned to the higher atoms.

Recommended Text: **The Elements of Physical Chemistry** - *P. W. Atkins*, *J. de Paula*, 4th Ed, Oxford University Press (2005).

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This Atomic Structure Unit is delivered in seven sessions which are:

Session 1: The electronic structure of atoms
Session 2: Behaviour Of The Electron In The Constant Energy Hydrogen Atom
Session 3: The Schrödinger Wave Equation and the Ground & Excited States of Hydrogen
Session 4: Quantum Numbers
Session 5: The Electronic Structure of Higher Atoms
Session 6: Spherical Polar Coordinates, Radial & Angular Wavefunctions
Session 7: Angular Momentum & Space Quantization and Ionization Enthalpies

In this unit we will be looking at the behaviour of the electron in the ground state hydrogen atom and will describe the behaviour in terms of its wave properties. We then look at the behaviour of the electron in excited states of hydrogen and explain the behaviour and properties of many-electron atoms by applying the information gained from hydrogen.

Learning objectives

At the end of this unit you will be able to:

- Calculate the electrostatic and gravitational forces between two bodies or particles
- State the Heisenberg Uncertainty Principle and calculate the uncertainty in position or velocity of a particle or body
- Define the de Broglie wavelength and calculate same for particles and bodies
- Explain interference and diffraction in light and electrons
- Explain the terms wavefunction, Eigenfunction and Hamiltonian operator as they appear in the Schrödinger Wave Equation
- Sketch the radial wavefunctions for the 1s, 2s and 2p orbitals
- Sketch the Radial Distribution Functions for 1s, 2s and 2p orbitals
- Define and depict radial and angular nodes on orbitals
- Define and give examples of principal, orbital angular momentum, magnetic and spin quantum numbers
- Calculate the energy of the levels and the emission lines in the hydrogen atom
- Explain the Orbital Approximation and apply it to the Helium atom
- State the Pauli Exclusion Principle, and rationalize it in terms of the relative stability of different electronic configurations (e.g. Lithium).

- State Hund's rule and explain it in terms of the relative stability of the different electronic configurations of sub-shells (e.g. Carbon)
- Define Cartesian and Spherical Polar coordinates
- State advantages of expressing wavefunctions in Spherical Polar coordinates
- Define radial wavefunction and angular wavefunction
- Calculate and plot the hydrogen **1s** Radial wavefunction
- Define and calculate orbital angular momentum of an electron in different orbitals
- Define and explain Space Quantization
- Define Ionization Enthalpy and explain its trend across the Li – Ne period.