Chapter 7 - The Quantum Mechanical Model of the Atom

Section 7.1 - ELECTROMAGNETIC RADIATION

1. **Electromagnetic radiation -** the way energy travels through space.
2. **Wavelength (λ) -** the distance between two consecutive peaks or troughs in a wave.
3. **Frequency (ν) -** the number of waves (cycles) per second that pass a given point in space.

****<u>Note</u>**** Wavelength and frequency are inversely related.

$$l n = c \qquad\qquad c = \text{speed of light} = 2.9979 \times 10^{8} \text{ m/s}$$

Section 7.2 - Nature of Matter

1. **Planck's constant (*h*) -** the quantity of energy that can be absorbed or emitted. ***h*** = 6.626 x 10-34 J•s

Now the energy of a system **ΔE** (as we learned last chapter) can be defined as

$$\Delta E = nhn$$

where ***n*** is an integer, ***h*** is Planck's constant and **ν** is the frequency of the electromagnetic radiation absorbed or emitted.

2. **Energy** is in fact **quantized** and can only occur in discrete units of size ***hv***. Each of these small "packets" of energy is called a **quantum** (or a **photon** when we are talking about light).

$$E_{\text{photon}} = hv = \frac{hc}{l}$$

Einstein at the same time came up with the idea that **E** (energy) has mass (***m***). Giving us the equation

$$E = mc^2$$

3. **Dual nature of light -** phenomenon in which light acts like both a wave and a particle of matter. The previous two equations were used by deBroglie to form the following equation to help confirm this idea of duality electromagnetic radiation.

$$m = \frac{h}{l\,\text{v}} \quad \text{or rearranged} \quad l = \frac{h}{m\text{v}}$$ where ***m*** = mass, and **v** = velocity.

4. **Diffraction and diffraction pattern -** when light is scattered from a regular array of points or lines.
5. **Conclusion -** Energy is really a form of matter, and all matter shows the same types of properties. That is, all matter exhibits both particulate and wave properties. Large pieces of matter, such as baseballs, exhibit predominantly particulate properties. The associated wavelength is so small that it is not observed. Very small bits of matter, such as photons, while showing some particulate properties, exhibit predominantly wave properties. Pieces of matter intermediate mass, such as electrons, show clearly both the particulate and wave properties of matter.

Section 7.3 - THE ATOMIC SPECTRUM OF HYDROGEN

1. **Continuous spectrum -** this spectrum results when white light passes through a prism, like the rainbow produced when sunlight is dispersed by raindrops, it contains all the wavelengths of visible light.
2. **Line spectrum -** in this spectrum , we see only a few lines, each of which corresponds to a discrete wavelength. The significance of the line spectrum is that it indicates that only certain energies are allowed for the electron in the atom.

Section 7.4 - The Bohr Model

1. **Quantum model -** the electron in a hydrogen atom moves around the nucleus only in certain allowed circular orbits. The equation used to express the energy levels available to the electron in the hydrogen atom is:

$$E = -2.178 \times 10^{-18}\ \mathrm{J}\left(\frac{Z^2}{n^2}\right)$$

2. **Ground state -** lowest possible energy for an electron. The wavelength of the emitted photon can be calculated from the equation:

$$l = \frac{hc}{\Delta E}$$

Section 7.5 - The Quantum Mechanical Model

1. **Quantum Mechanics -** broke away from the traditional particulate models and offered wave mechanics as the basis of describing electrons in an atom.
2. **Standing wave -** stationary waves, which do not travel along the length of the string. Like musical instruments.
3. **Wave function (ψ) -** a function of the coordinates (x, y, and z) of the electron's position in three-dimensional space.
4. **Orbital -** a specific wave function (we called it an area of high probability).
5. **Heisenberg uncertainty principle -** a fundamental limitation to just how precisely we can know both the position and momentum of a particle at a given time.

$$\Delta x \cdot \Delta(mv) \geq \frac{h}{4p}$$

Where **Δx** is the uncertainty in a particle's position, **Δ(mv)** is the uncertainty in a particle's momentum, and ***h*** is Planck's constant.
The square of the wave function indicates the probability of finding an electron near a particular point in space.

6. **Probability distribution -** the way the square of the wave function is most conveniently represented, in which intensity of color is used to indicate the probability value near a given point.
7. **Electron density map -** a graphical representation (diagram) of the electrons probability distribution. The darkness of a point indicates the probability of finding an electron at that position.

Section 7.6 - Quantum Numbers

1. **Quantum numbers -** each of the orbitals are characterized by a series of numbers which describe various properties of the orbital.

   A. **Principal quantum number (n) -** has integral values: 1, 2, 3, … related to the size and energy of the orbital.
   B. **Angular momentum quantum number (l) -** has integral values from 0 to n - **l** for each value of n. Related to the shape of atomic orbitals. (subshell)
   C. **Magnetic quantum number (m_l) -** has integral values between **l** and - **l** including zero. Related to the orientation of the orbital in space relative to the other orbitals in the atom.

Section 7.7 - Orbital Shapes and Energies

Nodal surfaces (nodes) - areas of zero probability in between areas of high probability. (Remember standing waves?)

Summary of the hydrogen Atom

1. In the quantum (wave) mechanical model, the electron is viewed as a standing wave. This representation leads to a series of wave functions (orbitals) that describe the possible energies and spatial distributions available to the electron.
2. In agreement with the Heisenberg uncertainty principle, the model cannot specify the detailed electron motions. Instead, the square of the wave function represents the probability distribution of the electron in the orbital. This allows us to picture orbitals in terms of probability distributions, or electron density maps.

3. The size of an orbital is arbitrarily defined as the surface that contains 90% of the total electron probability.
4. The hydrogen atom has many types of orbitals. In the ground state, the single electron resides in the 1s orbital. The electron can be excited to higher-energy orbitals if energy is put into the atom.

Section 7.8 - Electron Spin and the Pauli Principle

1. **Electron spin (m_s) -** the fourth quantum number, developed by Goudsmit and Uhlenbeck, was necessary to account for the details of the emission spectra of atoms. The spectra indicated that the electron had a magnetic moment with two possible orientations. Has values of + ½ and **-** ½.
2. **Paulie exclusion principle -** in a given atom no two electrons have the same set of four quantum numbers.

Section 7.9 - Polyelectronic Atoms

1. **Polyelectronic atoms -** atoms with more than one electron. A problem occurs when you apply Schrödingers equation to polyelectronic atoms, results cannot be solved exactly. Electron repulsion seems to be the problem. This is called the electron correlation problem. So approximations must be made to simplify the problem.
2. Outer electrons are not held as strongly to the nucleus do to **shielding**, the repulsion of the inner electrons on the outer electrons, causing weaker attraction to the nucleus.
3. **Energy of the sublevels -** energy increases in this manner.

$$E_{ns} < E_{np} < E_{nd} < E_{nf}$$

4. **Penetration effect -** allows, for example, 2s electrons to be more strongly attracted to the nucleus than 2p electrons. Thus 2s electrons have lower energy than 2p electrons.

Section 7.11 - Aufbau Principle and the Periodic Table

1. **Aufbau principle -** as protons are added one by one to the nucleus to build up the elements, electrons are similarly added to these hydrogen-like orbitals.
2. **Electron configuration** and **Orbital notation (Orbital diagram)**
3. **Hund's rule -** the lowest energy configuration for an atom is the one having the maximum number of unpaired electrons allowed by the Pauli principle in a particular set of degenerate (same energy) orbitals.
4. **Valence electrons -** the electrons in the outermost principal quantum level of an atom.
5. **Core electrons -** inner electrons.
6. The elements in the same **group (family)** have the same valence electron configuration.
7. **International Union of Pure and Applied Chemistry (IUPAC) -** a body of scientists organized to standardize scientific conventions.

****Notes have been derived from Zumdahl 4th ed. - All page and table references are made to this edition.**