Atomic Structure

Atom - the smallest particle of an element that retains the properties of that element

Greek Model - Fourth and Fifth Centuries BC

- The word ***atom*** is from the Greek word ***atomos***, which means indivisible or uncut
- This was the original model of the atom
- It viewed the atom as the smallest indivisible particle of matter
- This theory was never verified by experiments and was discarded

Dalton's Atomic Theory - John Dalton (1766-1844)

1. All elements are composed of tiny indivisible particles called atoms.
2. Atoms of the same element are identical. The atoms of any one element are different from those of any other element.
3. Atoms of different elements can combine with another in simple whole number ratios to form compounds.
4. Chemical reactions occur when atoms are separated, joined, or rearranged. However, atoms of one element cannot be changed into atoms of another element by a chemical reaction.

Revisions to Dalton's Atomic Theory

Dalton believed that atoms were indivisible. Today we know that atoms can be broken down into smaller particles.

These particles are: ***electrons*** - negatively charged, ***protons*** - positively charged, and ***neutrons*** - neutral (no charge)

Joseph John Thomson (1856-1940)

J.J. Thomson discovered electrons while experimenting with cathode rays. A cathode ray is produced when a high voltage is applied to an electrode in a closed tube with a partial vacuum.

A glowing beam travels from the cathode to the anode. Thomson discovered that cathode rays could be deflected by magnets and/or charged plates. He also determined that cathode rays were identical regardless of which metal was used for the cathode.

From his results, J.J. Thomson concluded that electrons are part of the atoms of all elements and that all electrons are identical.

Thomson viewed the atom as a sphere of uniform positive charge with negative electron embedded throughout. This model was often called the "plum pudding model".

Rutherford's Model of the Atom (1871-1937)

In 1896 Henri Becquerel discovered radioactivity. Working with radium (a radioactive element) Rutherford discovered that the invisible rays were actually composed of three different rays: alpha (positively charged), beta (negatively charged), and gamma (uncharged) rays. These experiments were performed while Rutherford was the head of the physics department at McGill University in Montreal.

The Gold Foil Experiment

Using alpha particles, Rutherford investigated the scattering of these particles by thin sheets of gold foil. According to the Thomson model atoms are essentially a sphere of uniform positive charge with negative charges embedded throughout. If the positive charge of the atom is evenly distributed, and the electrons are spread out and have little mass, there should be nothing to prevent the fast alpha particles from passing through the gold foil unchanged.

Most of the alpha particles did pass through the gold foil undeflected, but some were deflected, while some were actually reflected. The Thomson model could not explain this result. Rutherford proposed his own model to account for these results.

Rutherford suggested that an atom had a ***nucleus*** or center in which the positive charge and most of the mass were located. This nucleus occupied only a tiny portion of the volume of the entire atom. The electrons were located outside the nucleus. This model of the atom is often called the "nuclear" atom.

The Bohr Model of the Atom

The nuclear model of the atom raised some questions. Why are the negative electron not pulled into the nucleus by the attraction of unlike charges?

Bohr studied the line spectrum of hydrogen. When hydrogen gas is excited (forced into a higher energy state) by an electric current it will emit energy in the form of visible light. If this light is passed through a prism, it separates into its component colours or frequencies. The line spectrum of hydrogen consists of four prominent coloured lines, each of which corresponds to a characteristic energy. Bohr believed that these lines were produced when an electron in the hydrogen atom jumped from a higher energy level to a lower energy level. He believed that the electrons orbit at fixed distances from the nucleus. This distance is known as an ***energy level***. Higher energy levels are located further from the nucleus. An electron is able to jump to a higher level by gaining the exact amount of energy required. When an electron drops to a lower energy level, the energy difference is released in the form of light. Bohr developed his theory based on the light given off by the electrons in hydrogen atoms.

The Quantum Mechanical Model of the Atom

Bohr's model of the atom worked very well with hydrogen, which has only one electron per atom, however, problems arose when it was applied to atoms with more than one electron.

Erwin Schrödinger developed a mathematical equation describing the location and energy of the electrons in atoms. This equation works for hydrogen as well as atoms with more than one electron.

Similar to the Bohr model, the quantum mechanical model also places electrons in energy levels. It is different in the following ways:

The exact path of the electron cannot be defined, only the probability of the electron's location. This is described as an electron cloud. The electron can be found anywhere within the cloud, but is most likely to be found where the cloud is most dense.

Within energy levels, there are sublevels called ***orbitals***. At higher energy levels there are more than one type of orbital.

Energy Levels, Orbitals, and Electrons

n = energy level

- the 1st energy level has 1 type of orbital (s)
- the 2nd energy level has 2 types of orbitals (s, & p)
- the 3rd energy level has 3 types of orbitals (s, p, & d)
- the 4th energy level has 4 types of orbitals (s, p, d, & f)

- At each energy level there is only one s orbital.
- At the second energy level and higher, there are three p orbitals.
- At the third energy level and higher, there are five d orbitals.
- At the fourth energy level and higher, there are seven f orbitals.

<u>Electron Configurations</u> - describes how the electrons are arranged in the atom.

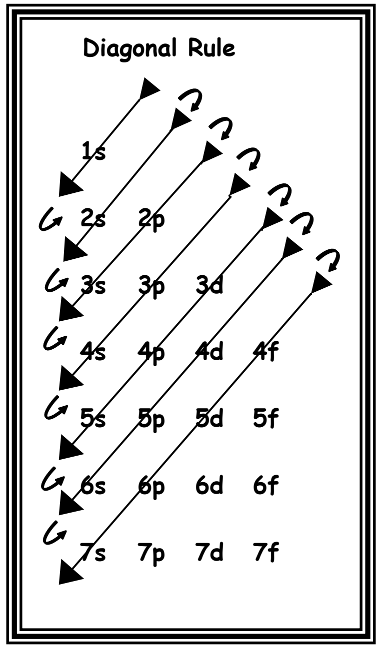
<u>Energy Level Diagram</u> – a diagram that illustrates how electrons are arranged in the atom.

<u>Energy Level Population</u> – states the number of electrons present at each energy level in an atom.

How Electrons are Arranged in Atoms

- <u>Aufbau Principle</u>: Electrons fill the lowest energy level orbitals first before entering higher energy orbitals.
- <u>Pauli Exclusion Principle</u>: An atomic orbital may contain zero, one, or two electrons. If two electrons occupy the same orbital, they must have opposite spin.
- <u>Hund's Rule:</u> When electrons enter orbitals of equal energy, each electron enters a separate orbital until all orbitals at the same energy are half full before any electrons pair up in the same orbital.

<u>Diagonal Rule</u> - Shows the order in which electrons enter orbitals.
- Shows how energy levels overlap.



<u>Quantum Numbers</u>
The Schrödinger equation is the central equation of the quantum theory. This equation correctly predicts the properties of multielectron atoms and molecules. When the Schrödinger equation is solved, we find that the energy of an electron is restricted to a discrete set of values, as in the Bohr theory; however, they differ in their description of the location of the electrons. Instead of restricting the electron to certain, sharp orbits, the Schrödinger equation provides one or more wave functions or orbitals associated with each allowed energy. The square of the wave function is a probability density. This represents the region where the probability of finding an electron is the greatest.

Each electron in an atom can be identified by its own set of four quantum numbers.

<u>Principal Quantum Number (n)</u> corresponds to the energy levels (1,2,3, …)

<u>Azimuthal Quantum Number (l)</u> specifies the shape of an orbital. ***l*** is restricted to the values 0, 1, … , ***n***-1. For historical reasons, the values of ***l*** are designated by letters: 0 = ***s***, 1 = ***p***, 2= ***d***, 3 = ***f***, … The letters ***s***, ***p***, ***d***, and ***f***, stand for ***s***harp, ***p***rincipal, ***d***iffuse, and ***f***undamental, for ***l*** = 4 and greater, the letters follow alphabetical order after ***f***.

<u>Magnetic Quantum Number (m)</u> determines the spatial orientation of an orbital. ***m*** is restricted to values from ***l*** to –***l***.

<u>Spin Quantum Number (s)</u> An electron spins like a top in one of two directions about its axis. The spin state of an electron can have one of two possible values: $\frac{1}{2}$ or $-\frac{1}{2}$.