Script Modern Atomic Theory

Part 1

Welcome to our presentation on modern atomic theory. This presentation is designed to enhance our understanding of atoms and their properties.

In the early 20 th century Neils Bohr proposed his model of the atom. In the Bohr model electrons circle the nucleus in predictable orbits, each orbit has a fixed size and energy level. However, Bohr's model was flawed. It turns out that electrons have wave-particle duality and we cannot know an electron's positon and velocity at the same time. Because we cannot know both of these things simultaneously it is impossible to predict an electron's exact trajectory, we can only create a probability distribution of where an electron is likely to be found.

Erwin Schrodinger refined Bohr's model using mathematical equations to predict an electron's probability of being in a certain position at any time. The space described by an electron's probability distribution is an orbital.

The probability density of an electron decreases as the distance from the nucleus increases. This means the likelihood of finding an electron is highest closer to the nucleus. Try not to get bogged down in the background explanation, for now understand that an orbital is a defined volume in space around a nucleus where an electron is likely to be found. There are equations that precisely describe the energy and shapes of the orbitals but practically, we can use a series of parameters, known as quantum numbers to summarize and describe our orbitals. So, for our purposes, each orbital can be described by a set of quantum numbers, and each quantum number has rules that define what values it can take.

The principle quantum number, n, describes an orbital's size and the energy level of the electron in the orbital. It's a whole number starting at one. Permitted values of n are: one, two, three and so on. An electron's energy and distance from the nucleus increases with increasing value of n, n is commonly known as a shell.

The angular momentum quantum number, *l,* corresponds to the shape of the orbital. It has permitted values that start at zero and increase to n minus one. So if n is two than *l* can be zero or one. The combination of n and *l* describe the energy level of the electron. (l) is often referred to as a subshell.

The value of *l* is assigned a letter, for example zero corresponds to s, one is p, two is d, three is f, 4 is g. You may recognise these letters as the labels used for orbitals.

The magnetic quantum number *m* sub *l* indicates the orientation of the orbital in space. There are two times *l* plus one values for each value of *l* and each value can be any integer from negative *l* to positive *l.* For example, If *l* is 0, m sub *l* is zero. If *l* is one, m sub *l* values are: -1,0,1.

Now that we have an understanding of quantum numbers we need to look at some orbital shapes. Remember that the shapes of orbitals correspond to the angular momentum number *l*. Let's look at some of the shapes of the orbitals defined by *l,* and the orbital's orientation in space described by m sub *l.* Orbitals are orientated in 3-D space defined using an x, y and z axis.

Part 2

For the s orbitals *l* equals zero, therefore m sub l has only one permitted value, zero. This means that for any one value of *n*, there is only one type of s orbital.

For all p orbitals *l* equals one, m sub *l* may have three values, one, zero, and negative one. This means that there are three types of p orbital for each value of *n* greater than and equal to two.

The d orbitals have an *l* value of two, m sub *l* has five values, therefore there are five d orbitals for each value of n greater than and equal to three.

These quantum numbers are the set of parameters required to completely describe an orbital, however, we need one more quantum number to completely describe an electron. The spin quantum number m sub s relates to the spin of an electron. Spin is an intrinsic property of all electrons, it is quantised, and there are only two possible alignments of spin, spin up and spin down. Designated as positive one half and negative one half. The spin quantum number leads to the Pauli Exclusion Principle which states that no two electrons in an atom can have the same four quantum numbers, but any three quantum numbers can be the same. This means one orbital must contain two electrons. A simple way of looking at quantum numbers is to think of it as an electron's address. The four numbers unique to each electron tell you where that electron can be found in an atom.

In a one electron system the subshells are degenerate; meaning s,p,d,f,.., all have the same energy level in each shell. However, in a multi-electron atom the subshells have different energy levels. We are usually interested in the lowest energy state that an atomic system can be in, this is known as its ground state.

That means that we want to know about a system in which the lower energy orbitals fill before the higher energy orbitals. This idea is referred to as the Aufbau principle, and the general order in which electrons fill orbitals in an atom to achieve the ground state configuration is:

1s,2s,2p,3s,3p,4s,3d,4p,5s,4d,5p,6s,4f,5d,6p,7s,5f,6d,7p

We just have one more concept to discuss before we complete our picture of quantum numbers, and that is Hund's rule. Hund's rule states that electrons will singly occupy

degenerate orbitals until they are all half full before pairing up with another electron; electrons occupying half full orbitals will all have the same spin.

Part 3

There are two ways we can use these rules to describe electrons in an atom. The first is electron configuration, a description of which orbitals are occupied by electrons in an atom. To write an electron configuration start by writing the value for n, followed by the letter value of *l* then as a superscript, the number of electrons that can be in each type of orbital. In carbon an atom with six electrons, the electron configuration is: $1s^2 2s^2 2p^2$.

Electron configurations become long to write when atoms have a lot of electrons. The use of a shorthand configuration is common. To write the shorthand configuration we need to know the difference between core electrons and valence electrons. Core electrons are those in the filled inner shells of an atom. The valence electrons are the electrons in the outermost shell, the highest n value, the valence electrons largely determine an atom's chemical behavior, and the short form electron configuration highlights the valence electrons. When writing a shorthand configuration a substitution for the core electrons is used, which is the previous noble gas in square brackets. For Carbon the shorthand configuration is [He] $2s^2\ 2p^2$.

Electron configurations do not give any information about the magnetic quantum number or spin of the electron, so we use orbital diagrams, the second way to describe electrons in an atom, to extract this information. In orbital diagrams each shell is represented as a line or a circle, then filled with arrows pointing up or down to represent the spin of an electron. For carbon we can fill the orbitals from the lowest energy level to the highest. The electrons in the p orbitals are not paired according to Hund's rule. An easy way to remember how the orbitals fill is to think of electrons as being lazy. It costs an electron energy to pair up or move to a higher level.

We have now covered the concepts of modern atomic theory. For a detailed tutorial on writing electron configurations watch the electron configurations and orbital diagram video included in this section. Work through the quantum number examples that have full solutions provided. You should now have a working knowledge of the atom and be able to define the terms: orbital, principle quantum number, angular momentum quantum number, magnetic quantum number, and spin quantum number. You should be able to recognise a set of allowed quantum numbers, and understand the Pauli Exclusion Principle, the Aufbau Principle and Hund's rule. You should be able to identify the shapes of the s, p, and d orbitals and define an electron configuration and orbital diagram.