

## Unit 1, Lesson 02: The Quantum Mechanical Model of the Atom

### Prelude:

The number of protons in an atom determines the identity of that atom. It also determines the number of electrons that the atom will have when it is neutral.

**It is the number and arrangement of electrons in an atom that determines the atom's chemical and physical properties.**

So, how are the electrons arranged?

Our models of the atom have progressed with our knowledge of electrons and their arrangement:

1. **John Dalton:** no such thing as electrons
2. **J.J. Thomson:** electrons are embedded in a solid, positively charged matrix
3. **Ernest Rutherford:** electrons are found flying rapidly and randomly around the nucleus in an electron cloud
4. **Neils Bohr** (applying Max Planck's idea of quantized energy): electrons move around the nucleus in defined, predictable orbits that have certain discrete energy levels called "quantum levels". All electrons in a given quantum level are exactly the same distance from the nucleus so they have exactly the same energy.

Bohr based his model of the atom on hydrogen, which has only a single electron.

For atoms that have more than two electrons, the electron-electron repulsion and wave-like behaviour of electrons mean that:

- electrons in a given quantum level do NOT travel in fixed, predictable orbits
- all electrons in a given quantum level are NOT exactly the same distance from the nucleus

We need a way to describe both an electron's energy (distance from the nucleus or "quantum level") and how it is moving (its "mechanics"). The stage is set for the "Quantum Mechanical Model".

5. **de Broglie (1924)** proposed that all matter has wave-like properties. For large objects, the wave-like properties are negligible, but for tiny particles like electrons, the wave-like motion is significant. This means that the motion of electrons is more complex than a simple orbit.
6. **Schrödinger (1926)** applied de Broglie's wave motion of particles and Planck/Einstein's idea of quantized energy particles (photons) to develop a mathematical model which predicts the motion of electrons around the nucleus of an atom. Schrödinger called this the "Quantum Mechanical Model" of the atom.
7. **Heisenberg (1927)** realized that we never know exactly where an electron is going to be. Remember, electrons are tiny. If we design an experiment to measure an electron's energy, we will alter the electron's motion (path or trajectory). If we design an experiment to see where an electron is going, we will change its energy. By measuring one, we change the other. That is, we can never know BOTH where an electron is, and how much energy that electron has.

**Heisenberg's Uncertainty Principle:** it is impossible to know both an electron's position and trajectory (where it is going).

## The Quantum Mechanical Model

(p. 131 – 133, 137 – 138)

Schrödinger incorporated the ideas of each of these researchers into the Quantum Mechanical Model of the atom. Basically, Schrödinger developed some pretty fancy math (called “wave functions”) to predict where the electrons in an atom are going to be found, 95% of the time. He called these regions “orbitals”.

An **orbital** is defined as a region in three-dimensional space where there is greater than a 95% probability that an electron will be found. An orbital can hold a maximum of two electrons. Orbitals are entirely different from orbits. If an object is moving in an orbit- we know exactly where it is going to be at all times. An orbital does not tell us where an electron is, only an area where we are likely to find it, 95% of the time.

So, Schrödinger divided Bohr’s principal quantum levels (n) into sub-levels containing one type of orbital (s, p, d, f etc). The principal quantum level and sub-level (type of orbital) indicate how far the electron is from the nucleus (its energy).

The shape of the orbital is defined by the motion of the electrons in that orbital. Within an orbital, there are a maximum of two electrons, with opposite spin ( $\uparrow\downarrow$ ). The shape of the orbital and spin of the electrons indicate the electron’s motion (its mechanics).

In order to describe both an electron’s energy (distance from the nucleus) and how it is moving, we use:

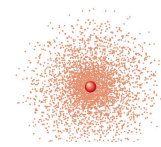
1. electron configurations
2. orbital diagrams
3. quantum numbers
4. electron density probability graphs which allow us to visualize a “size” and “shape” for the orbitals.

In this course, we will use electron configurations, orbital diagrams and quantum numbers to describe the energy and motion of electrons. You will use electron density probability graphs in university.

## Summary of the Quantum Mechanical Model

For **n = 1** (the \_\_\_\_\_ quantum level, or the energy level closest to the nucleus)

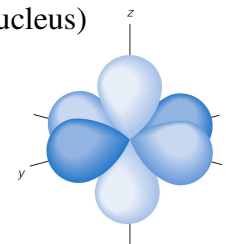
- holds a maximum of  $2n^2$  electrons, or ( ) \_\_\_\_\_ electrons
- there are  $n^2$  ( ) or \_\_\_\_\_ orbital (each orbital can hold 2 electrons)
- there is \_\_\_\_\_ (n) type of orbital:  
\_\_\_\_\_ spherical “s” orbital, called \_\_\_\_\_



an “s” orbital

For **n = 2** (the \_\_\_\_\_ quantum level, or the second energy level away from the nucleus)

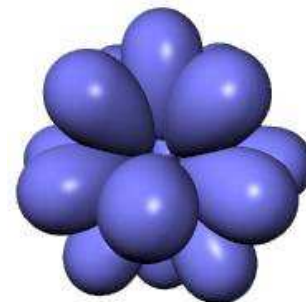
- holds a maximum of  $2n^2$  electrons, or ( ) \_\_\_\_\_ electrons
- there are  $n^2$  ( ) or \_\_\_\_\_ orbitals (each orbital can hold 2 electrons)
- there are \_\_\_\_\_ (n) types of orbitals:  
\_\_\_\_\_ spherical “s” orbital, called \_\_\_\_\_  
\_\_\_\_\_ perpendicular “p” orbitals called \_\_\_\_\_, \_\_\_\_\_ and \_\_\_\_\_  
(“p” orbitals are \_\_\_\_\_ shaped and found at right angles to each other in three three planes)



three “p” orbitals

For **n = 3** (the \_\_\_\_\_ quantum level)

- holds a maximum of  $2n^2$  electrons, or ( ) \_\_\_\_\_ electrons
- there are  $n^2$  ( ) or \_\_\_\_\_ orbitals (each orbital can hold 2 electrons)
- there are \_\_\_\_\_ (n) types of orbitals  
\_\_\_\_\_ spherical “s” orbital, called \_\_\_\_\_  
\_\_\_\_\_ perpendicular “p” orbitals called \_\_\_\_\_  
\_\_\_\_\_ diffuse “d” orbitals called \_\_\_\_\_  
(“d” orbitals are large, \_\_\_\_\_ shaped and found in five planes)



five “d” orbitals

For **n = 4** (the fourth quantum level, or the fourth energy level away from the nucleus)

- holds a maximum of  $2n^2$  electrons, or ( ) \_\_\_\_\_ electrons
- there are  $n^2$  ( ) or \_\_\_\_\_ orbitals (each orbital can hold 2 electrons)
- there are \_\_\_\_\_ (n) types of orbitals:  
\_\_\_\_\_ spherical “s” orbital, called \_\_\_\_\_  
\_\_\_\_\_ perpendicular “p” orbitals called \_\_\_\_\_  
\_\_\_\_\_ diffuse “d” orbitals called \_\_\_\_\_  
\_\_\_\_\_ fundamental “f” orbitals called \_\_\_\_\_ (the “f” orbitals are large, shape unknown)

There are an \_\_\_\_\_ number of quantum levels; each one is further and further from the nucleus. The types of orbitals are: \_\_\_\_\_ etc. The g, h, i etc. orbitals are for electrons in their \_\_\_\_\_.

### Question Types:

1. The maximum number of electrons that can be held in each quantum level is \_\_\_\_\_.
2. The total number of orbitals in each quantum level is \_\_\_\_\_.
3. The number of types of orbitals (sub-levels) in each quantum level is \_\_\_\_\_.
4. The types of orbitals are identified with letters . . . s, p, d, f, ...

If these occur in a given energy level there is(are) always:

\_\_\_\_\_ s-orbitals, \_\_\_\_\_ p-orbitals, \_\_\_\_\_ d-orbitals, \_\_\_\_\_ f-orbitals

5. The maximum number of electrons which may be designated (named):

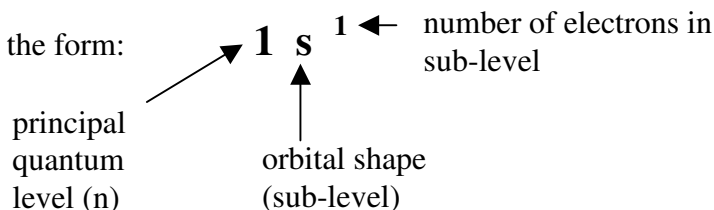
1s: \_\_\_\_\_, 2s: \_\_\_\_\_, 2p: \_\_\_\_\_, 3s: \_\_\_\_\_, 3p: \_\_\_\_\_, 3d: \_\_\_\_\_, 4s: \_\_\_\_\_, 4p: \_\_\_\_\_, 4d: \_\_\_\_\_, 4f: \_\_\_\_\_

## Electron Configurations

There are three rules when writing electron configurations:

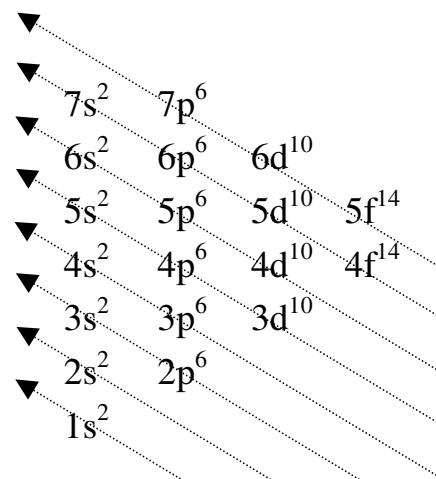
1. **Aufbau Principle:** electrons fill the lowest available energy level (get as close to the nucleus as possible)
2. **Pauli Exclusion Principle:** each orbital holds a maximum of two electrons with opposite spin
3. **Hund's Rule:** electrons do not pair up in an orbital until all orbitals of a certain sub-level are half-filled

Electron configurations are written using the form:



The order of filling puts the electrons as close to the nucleus as possible. The order of filling can be read from the periodic table or remembered using the mnemonic:

$_{15}\text{P}$  \_\_\_\_\_  
 $_{40}\text{Zr}$  \_\_\_\_\_  
 $_{76}\text{Os}$  \_\_\_\_\_  
 \_\_\_\_\_  
 \_\_\_\_\_



### Electron Configurations using the Condensed Format

Electron configurations can also be written using a “Condensed Format”. The non-valence electrons (electrons in full shells) are represented by the symbol of the nearest preceding Noble Gas, enclosed in square brackets, followed by the electron configurations for the valence electrons in the outer energy level.

Examples:

Standard Format		Condensed Format
$_{1}\text{H}$	$1s^1$	$1s^1$
$_{2}\text{He}$	$1s^2$	$1s^2$
$_{3}\text{Li}$	$1s^2 2s^1$	$[\text{He}] 2s^1$
$_{4}\text{Be}$	$1s^2 2s^2$	$[\text{He}] 2s^2$
$_{5}\text{N}$	$1s^2 2s^2 2p^3$	$[\text{He}] 2s^2 2p^3$
$_{8}\text{O}$	$1s^2 2s^2 2p^4$	$[\text{He}] 2s^2 2p^4$
$_{16}\text{S}$	$1s^2 2s^2 2p^6 3s^2 3p^4$	$[\text{Ne}] 3s^2 3p^4$
$_{18}\text{Ar}$	$1s^2 2s^2 2p^6 3s^2 3p^6$	$[\text{Ne}] 3s^2 3p^6$
$_{37}\text{Rb}$	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^1$	$[\text{Kr}] 5s^1$
$_{56}\text{Ba}$	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2$	$[\text{Xe}] 6s^2$
$_{86}\text{Rn}$	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^{10} 6p^6$	$[\text{Xe}] 6s^2 4f^{14} 5d^{10} 6p^6$

## Exceptions to the Predicted Electron Configurations

Electron configurations are used to explain and predict the chemical reactivity of the elements. There are some elements that do not behave according to their predicted electron configurations. Electrons always move into positions around the nucleus where they have the lowest energy. Electrons arrange themselves as close to the nucleus, but as far from each other, as possible. It turns out that when the “d” orbitals are half-filled or completely filled, the electrons can drop closer to the nucleus. This means that it is lower energy, or more stable, when the “d” orbitals are half-filled or completely filled.

### Chromium and molybdenum:

Each of the elements have a predicted electron configuration ending in  $s^2d^4$ .

Because it is lower energy (more stable) when the ‘d’ orbitals are all half filled, one of the ‘s’ electrons is promoted (moved up) to the ‘d’ sub-level and the actual electron configuration is  $s^1d^5$ .

eg. Chromium’s predicted electron configuration is:  ${}_{24}\text{Cr } 1s^22s^22p^63s^23p^64s^23d^4$ .

Experimentally, we find that the actual electron configuration is  ${}_{24}\text{Cr } 1s^22s^22p^63s^23p^64s^13d^5$ .

### Copper, silver and gold:

Each of these elements has a predicted electron configuration ending in  $s^2d^9$ .

Because it is lower energy (more stable) when the ‘d’ orbitals are filled, one of the ‘s’ electrons is promoted (moved up) to the ‘d’ sub-level and the actual electron configuration is  $s^1d^{10}$ .

eg. Copper’s predicted electron configuration is:  ${}_{29}\text{Cu } 1s^22s^22p^63s^23p^64s^23d^9$ .

Experimentally, we find that the actual electron configuration is  ${}_{29}\text{Cu } 1s^22s^22p^63s^23p^64s^13d^{10}$ .