

# Inorganic Pharmaceutical Chemistry

Lecture No. 2

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## Quantum Numbers

The relation of a particular electron to the nucleus can be described through a series of four numbers, called the Quantum Numbers. The first three of these numbers describe the energy (Principle quantum number), shape (Angular momentum quantum number), and orientation of the orbital (magnetic quantum number). The fourth number represents the "spin" of the electron (spin quantum number). The four quantum numbers are described below.

1. Principal Quantum Number ( $n$ ):  $n = 1, 2, 3, \dots, \infty$   
Specifies the energy of an electron and the size of the orbital (the distance from the nucleus of the peak in a radial probability distribution plot). All orbitals that have the same value of  $n$  are said to be in the same shell (level). For a hydrogen atom with  $n=1$ , the electron is in its ground state; if the electron is in the  $n=2$  orbital, it is in an excited state.

Electrons are negatively charged, so electrons that are closer to the positively charged nucleus are more powerfully attracted and tightly bound than those that are farther away. Electrons that are closer to the nucleus are thus more stable, and less likely to be lost by the atom. In other words, as  $n$  increases, so does the energy of the electron and the likelihood of that electron being lost by the atom.

2 .The next quantum number, represented by  $l$  and called the "angular quantum number," can be any value in the range  $0, 1, 2, \dots, n - 1$ . Specifies the shape of an orbital with a particular principal quantum number. The secondary quantum number divides the shells into smaller groups of orbitals called sub shells (sublevels). Usually, a letter code is used to identify  $l$  to avoid confusion with  $n$ :

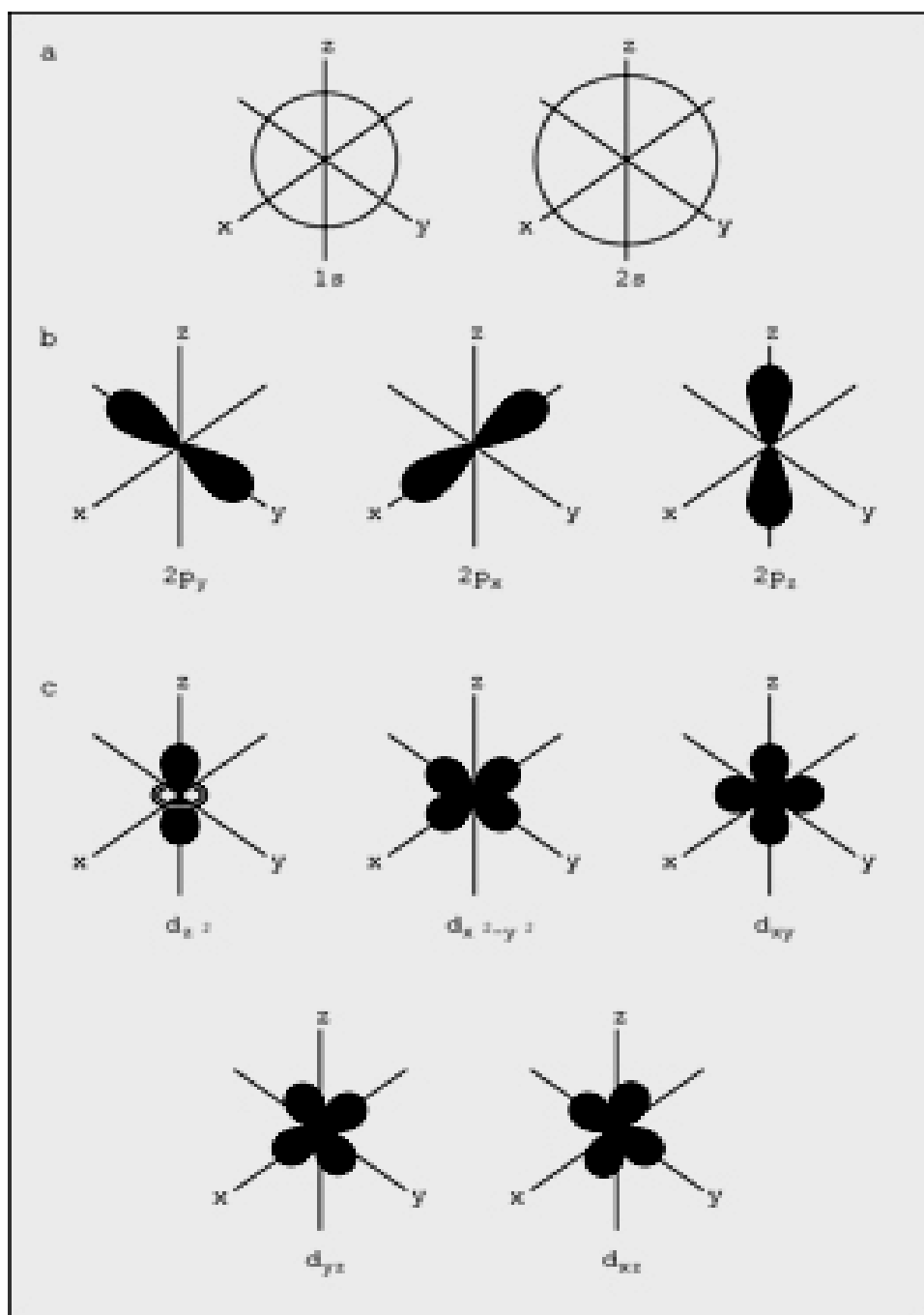
1	0	1	2	3	4	5	...
Letter s	p	d	f	g	h	...	

For example: when  $n = 1$ ,  $l$  can only equal 0; meaning that shell  $n = 1$  has only an s orbital ( $l = 0$ ). when  $n = 3$ ,  $l$  can equal 0, 1, or 2; meaning that shell  $n = 3$  has s, p, and d orbitals.

Another example : the sub shell with  $n=2$  and  $l=1$  is the 2p subshell; if  $n=3$  and  $l=0$ , it is the 3s subshell, and so on. The value of  $l$  also has a slight effect on the energy of the subshell; the energy of the subshell increases with  $l$  ( $s < p < d < f$ ).

The shapes of s orbitals are spherical, whereas p orbitals are dumbbell-shaped. d orbitals and beyond are much harder to visually represent.

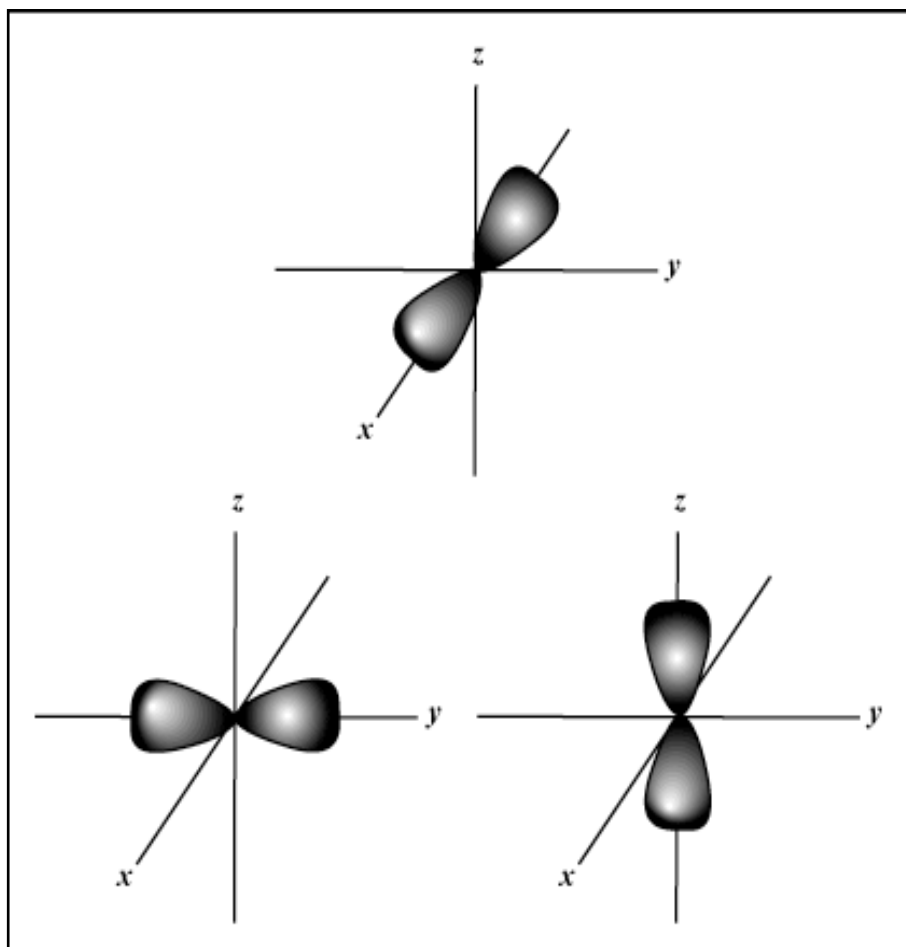
The following figure shows the shapes of the s, p, and d orbitals.



As shown in the top row of the figure (a), there are two s orbitals — one for energy level 1 (1s) and the other for energy level 2 (2s). The s orbitals are spherical with the nucleus at the center. Notice that the 2s orbital is larger in diameter than the 1s orbital. In large atoms, the 1s orbital is nestled inside the 2s, just like the 2p is nestled inside the 3p.

The second row of the figure (b) shows the shapes of the p orbitals, and the last two rows (c) show the shapes of the d orbitals. Notice that the shapes get progressively more complex.

3. The magnetic quantum number is designated as  $m_l = -l, \dots, 0, \dots, +l$ . Specifies the orientation in space of an orbital of a given energy (n) and shape (l). This number divides the subshell into individual orbitals which hold the electrons; there are  $2l+1$  orbitals in each subshell. For example, if the value of  $l = 1$  (p orbital), you can write three values for this number:  $-1, 0,$  and  $+1$ . This means that there are three different p subshells for a particular orbital. The subshells have the same energy but different orientations in space.



4. The fourth and final quantum number is the spin quantum number, designated as: ( $m_s$ ): Specifies the orientation of the spin axis of an electron. The spin quantum number describes the direction the electron is spinning in a magnetic field — either clockwise or counterclockwise. Only two values are allowed:  $+1/2$  or  $-1/2$ . For each subshell, there can be only two electrons, one with a spin of  $+1/2$  and another with a spin of  $-1/2$ .

## Electron Configurations

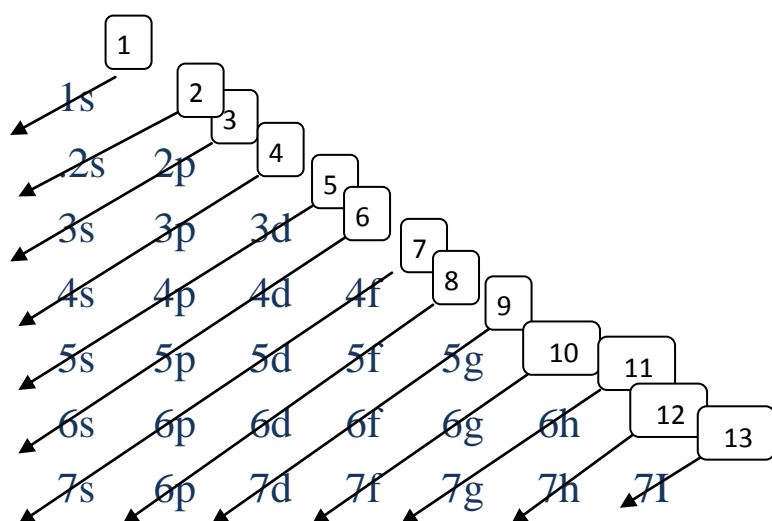
The electron configuration of an atom is the representation of the arrangement of electrons that are distributed among the orbital shells and subshells. Commonly, the electron configuration is used to describe the orbitals of an atom in its ground state, but it can also be used to represent an atom that has ionized into a cation or anion by compensating with the loss of or gain of electrons in their subsequent orbitals. Many of the physical and chemical properties of elements can be correlated to their unique electron configurations. The valence electrons, electrons on the outer most shell, become the determining factor for the unique chemistry of the element.

The electron configuration of each element is unique to its position on the periodic table. The energy level is determined by the period and amount of electrons by the atomic number of the element. Orbitals on different energy levels are similar to each other, but they occupy different areas in space. The 1s orbital and 2s orbital both have the characteristics of an s orbital (radial nodes, spherical volume probabilities, can only hold two electrons, etc.) but as they are found in different energy levels they occupy different spaces around the nucleus. Each orbital can be represented by specific blocks on the periodic table. The s-block is the region of the Alkali metals including Helium (groups 1 & 2), the d-block is the Transition metals (groups 3 to 12), the p-block are the main group elements from group 13 to 18, and the f-block are the Lanthanides and Actinides series.

Using the periodic table to determine the electron configurations of atoms is key, but also keep in mind that there are certain rules to follow when assigning electrons to different orbitals. The periodic table is an incredibly helpful tool in writing electron configurations.



One way to remember this pattern, probably the easiest, is to refer to the periodic table and remember where each orbital block falls to logically deduce this pattern. Another way is to make a table like the one below and use vertical lines to determine which subshells correspond to each other.



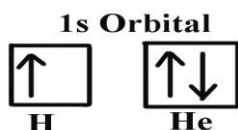
### Pauli Exclusion Principle

The second major fact to keep in mind is the Pauli Exclusion Principle **which states that no two electrons can have the same four quantum numbers**. (this means is that no more than two electrons can occupy the same orbital, and that two electrons in the same orbital must have opposite spins). The first three ( $n, l,$  and  $m_l$ ) may be similar but the fourth quantum number must be different. We are aware that in one orbital a maximum of two electrons can be found and the two electrons must have opposing spins. That means one would spin up ( $+1/2$ ) and the other would spin down ( $-1/2$ ). This tells us that each subshell has double the electrons per orbital. The s subshell has 1 orbital that can hold to 2 electrons, the p subsheel has 3 orbitals that can hold up to 6 electrons, the d subshell has 5 orbitals that hold up to 10 electrons, and the f subshell has 7 orbitals with 14 electrons.

Because an electron spins, it creates a magnetic field, which can be oriented in one of two directions. For two electrons in the same orbital, the spins must be opposite to each other; the spins are said to be paired. These substances are not attracted to magnets and are said to be diamagnetic. Atoms with more electrons that spin in one direction than another contain unpaired electrons. These substances are weakly attracted to magnets and are said to be paramagnetic

## Example

We have the first three quantum numbers  $n=1$ ,  $l=0$ ,  $m_l=0$ . Only two electrons can correspond to these, which would be either  $m_s = -1/2$  or  $m_s = +1/2$ . As we already know from our studies of quantum numbers and electron orbitals, we can conclude that these four quantum numbers refer to 1s subshell. If only one of the  $m_s$  values are given then we would have  $1s^1$  (denoting Hydrogen) if both are given we would have  $1s^2$  (denoting Helium). Visually this would be represented as:



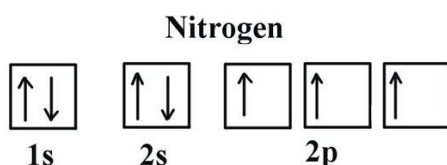
As you can see, the 1s subshell can hold only two electrons and when filled the electrons have opposite spins.

## Hund's Rule

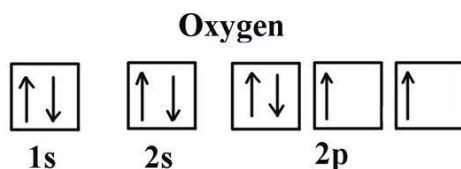
When assigning electrons in orbitals, **each electron will first fill all the orbitals with similar energy (also referred to as degenerate) before pairing with another electron in a half-filled orbital.** Atoms at ground states tend to have as many unpaired electrons as possible. When visualizing this processes, think about how electrons are exhibiting the same behavior as the same poles on a magnet would if they came into contact; as the negatively charged electrons fill orbitals they first try to get as far as possible from each other before having to pair up.

## Example

If we look at the correct electron configuration of Nitrogen ( $Z = 7$ ), a very important element in the biology of plants:  $1s^2 2s^2 2p^3$



We can clearly see that p orbitals are half filled as there are three electrons and three p orbitals. This is because Hund's Rule states that the three electrons in the 2p subshell will fill all the empty orbitals first before filling orbitals with electrons in them. If we look at the element after Nitrogen in the same period, Oxygen ( $Z = 8$ ) its electron configuration is:  $1s^2 2s^2 2p^4$



Oxygen has one more electron than Nitrogen and as the orbitals are all half filled the electron must pair up.

## The Aufbau Process

Aufbau comes from the German word "Aufbauen" which means "to build".

When writing electron configurations, we are building up electron orbitals as we proceed from atom to atom. As we write the electron configuration for an atom, we will fill the orbitals in order of increasing atomic number. However, there are some exceptions to this rule.

### Example

If we follow the pattern across a period from B (Z=5) to Ne (Z=10) the number of electrons increase and the subshells are filled. Here we are focusing on the p subshell in which as we move towards Ne, the p subshell becomes filled.

B (Z=5) configuration:  $1s^2 2s^2 2p^1$

C (Z=6) configuration:  $1s^2 2s^2 2p^2$

N (Z=7) configuration:  $1s^2 2s^2 2p^3$

O (Z=8) configuration:  $1s^2 2s^2 2p^4$

F (Z=9) configuration:  $1s^2 2s^2 2p^5$

Ne (Z=10) configuration:  $1s^2 2s^2 2p^6$