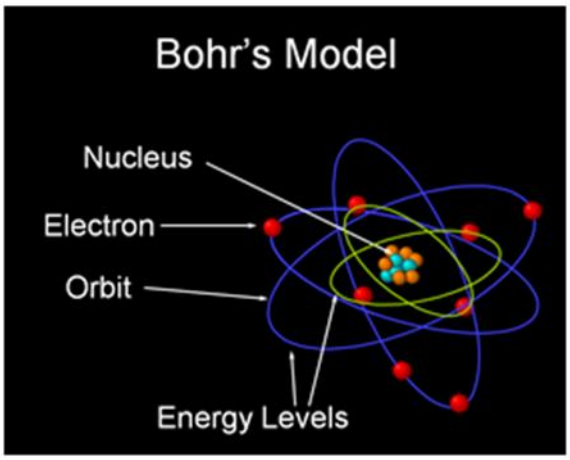
FARJANA YEASMIN
LECTURER, DEPT. OF FSE

INORGANIC CHEMISTRY

Bohr's atomic model

Rutherford's atomic model failed to answer many questions related to the energy of an atom and its stability. In the year 1913, Niels Bohr proposed an atomic structure model, describing an atom as a small, positively charged nucleus surrounded by electrons that travel in circular orbits around the positively charged nucleus as planets around the sun in our solar system, with attraction provided by electrostatic forces, popularly known as Bohr's atomic model. It was basically an improved version of Rutherford's atomic model overcoming its limitations. On most of the points, he is in agreement with him, like concepts of nucleus and electrons orbiting it. Salient features of Bohr's atomic model are:

1. Electrons revolve around the nucleus in stable orbits without emission of radiant energy. Each orbit has a definite energy and is called energy shell or energy level.
2. An orbit or energy level is designated as K, L, M, N shells. When the electron is in the lowest energy level, it is said to be in the ground state.



INORGANIC CHEMISTRY

3. An electron emits or absorbs energy when it jumps from one orbit or energy level to another. When it jumps from higher energy level to lower energy level it emits energy while it absorbs energy when it jumps from lower energy level to higher energy level.
4. The energy absorbed or emitted is equal to the difference between the energies of the two energy levels (E_1, E_2) and is determined by Plank's equation.

$$\Delta E = E_2 - E_1 = hv$$

Where,

ΔE = energy absorbed or emitted

h= Plank's constant

v= frequency of electromagnetic radiation emitted or absorbed

Angular momentum of an electron revolving in energy shells is given by:

$$m_e vr = \frac{nh}{2\pi}$$

Where,

n= number of corresponding energy shell; 1, 2, 3 …..

m_e= mass of the electron

v= velocity

r=radius

h= Plank's constant

INORGANIC CHEMISTRY

Limitations of Bohr Atomic Model Theory:

1. It violates the Heisenberg Uncertainty Principle. The Bohr atomic model theory considers electrons to have both a known radius and orbit i.e. known position and momentum at the same time, which is impossible according to Heisenberg.
2. The Bohr atomic model theory made correct predictions for smaller sized atoms like hydrogen, but poor spectral predictions are obtained when larger atoms are considered.
3. It failed to explain the Zeeman effect when the spectral line is split into several components in the presence of a magnetic field.
4. It failed to explain the Stark effect when the spectral line gets split up into fine lines in the presence of electric field.

Atomic Orbitals and Quantum Numbers

Orbit: Orbit is a well-defined by circular path around the nucleus in which an electron revolves. Orbit of definite energy levels called shells. These shells are named as K, L, M and N and numbered as 1, 2, 3 and 4 respectively from the nucleus. An orbit (shell) can accommodate electrons equal to $2n^2$.

For K shell, n=1

Maximum no of electrons in K shell=$2n^2 = 2(1)^2 = 2$

Therefore maximum no of e-s in K shell = 2

Similarly for L shell, n = 2, Therefore maximum no of e-s = 8

for M shell, n=3, Therefore maximum no of e-s =18

for N shell, n = 4, Therefore maximum no of e-s =32

INORGANIC CHEMISTRY

Orbital: Orbital is the three dimensional region around the nucleus where the probability of finding electron density is maximum. All orbitals have definite shape and each can accommodate maximum of two electrons in it. Orbital are named as s, p, d and f. s orbital can accommodate 2 electrons. There are three p orbital, each can accommodate two electrons therefore totally p orbital can accommodate 6 electrons. There are five d orbital so it can accommodate maximum of 10 electrons and there are seven f orbital and it can accommodate14 electrons.

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:

Principle Quantum Number (N)

The principle quantum number indicates how the distance of the orbital from the nucleus. Electrons are farther away for higher values of n. 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. In a given atom, all the atomic orbitals with the same n are collectively known as a shell. n can take on integer values of 1 or higher (ex. 1, 2, 3, etc.).

Angular Momentum Quantum Number (l)

The angular momentum quantum number describes the shape of the orbital. The angular momentum number (or subshell) can be represented either by a number (any integer from 0 up to n-1) or by a letter (s,p,d,f,g, and then up the alphabet), with 0 corresponding to s, 1 to p, 2 to d, andso on. 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.

s orbitals are spherical, whereas p orbitals are dumbbell-shaped. D orbitals and beyond are much harder to visually represent.

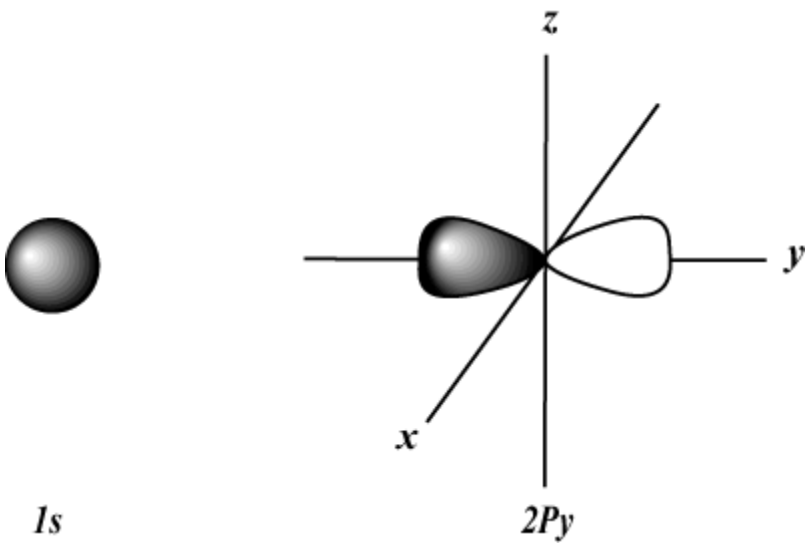


Figure : s and p atomic orbital shapes

INORGANIC CHEMISTRY

Magnetic Quantum Number (M)

Gives the orientation of the orbital in space; in other words, the value of m describes whether an orbital lies along the x-, y-, or z-axis on a three-dimensional graph, with the nucleus of the atom at the origin. m can take on any value from -l to l. For our purposes, it is only important that this quantum number tells us that for each value of n there may be up to one s-orbital, three p-orbitals, five d-orbitals, and so on. For example:

The s orbital (l = 0) has one orbital, since m can only equal 0. That orbital is spherically symmetrical about the nucleus.

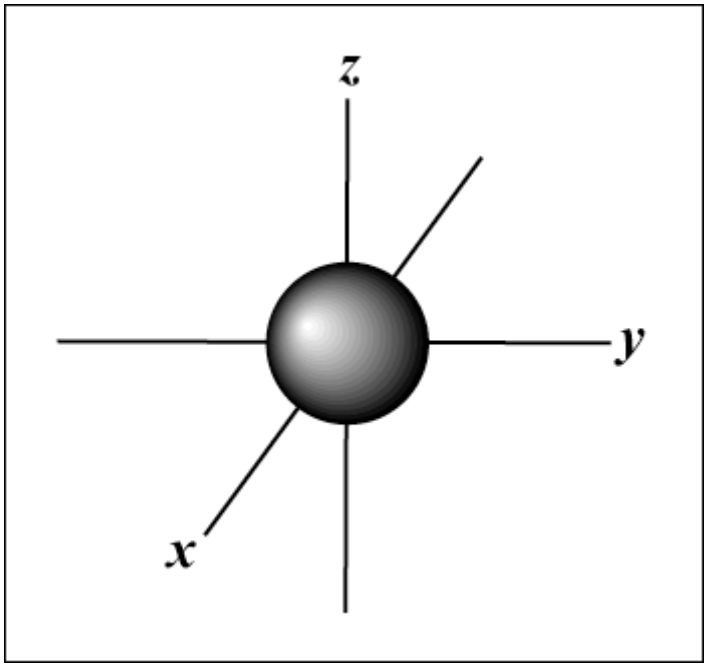


Figure : s orbital

The p orbital (l = 1) has three orbitals, since m = -1, 0, and 1. These three orbitals lie along the x-, y-, and z-axes.

INORGANIC CHEMISTRY

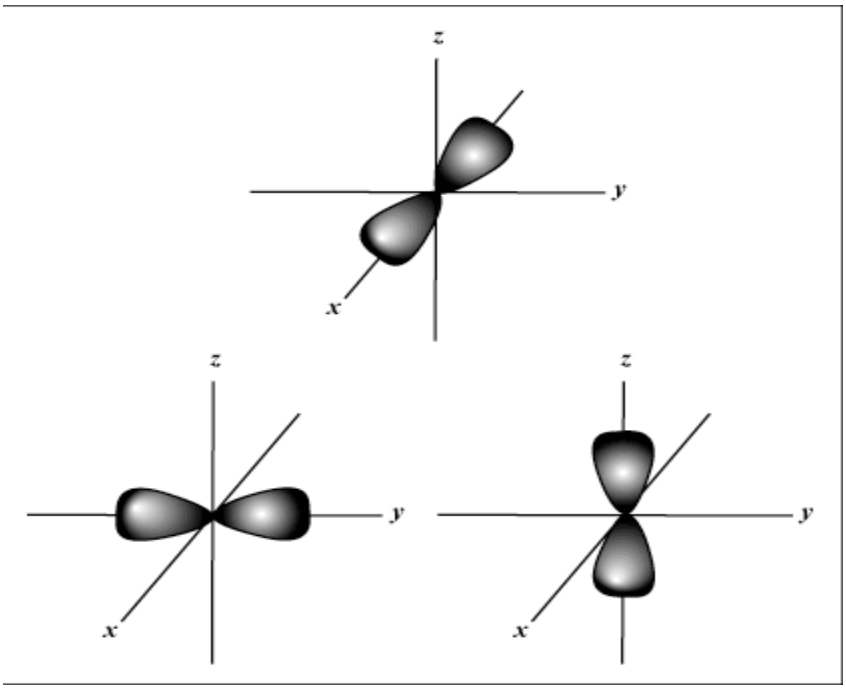


Figure %: p orbitals

The d orbital (l = 2) has five orbitals, since m = -2, -1, 0, 1, and 2. It is far more difficult to describe the orientation of d orbitals, as you can see:

INORGANIC CHEMISTRY

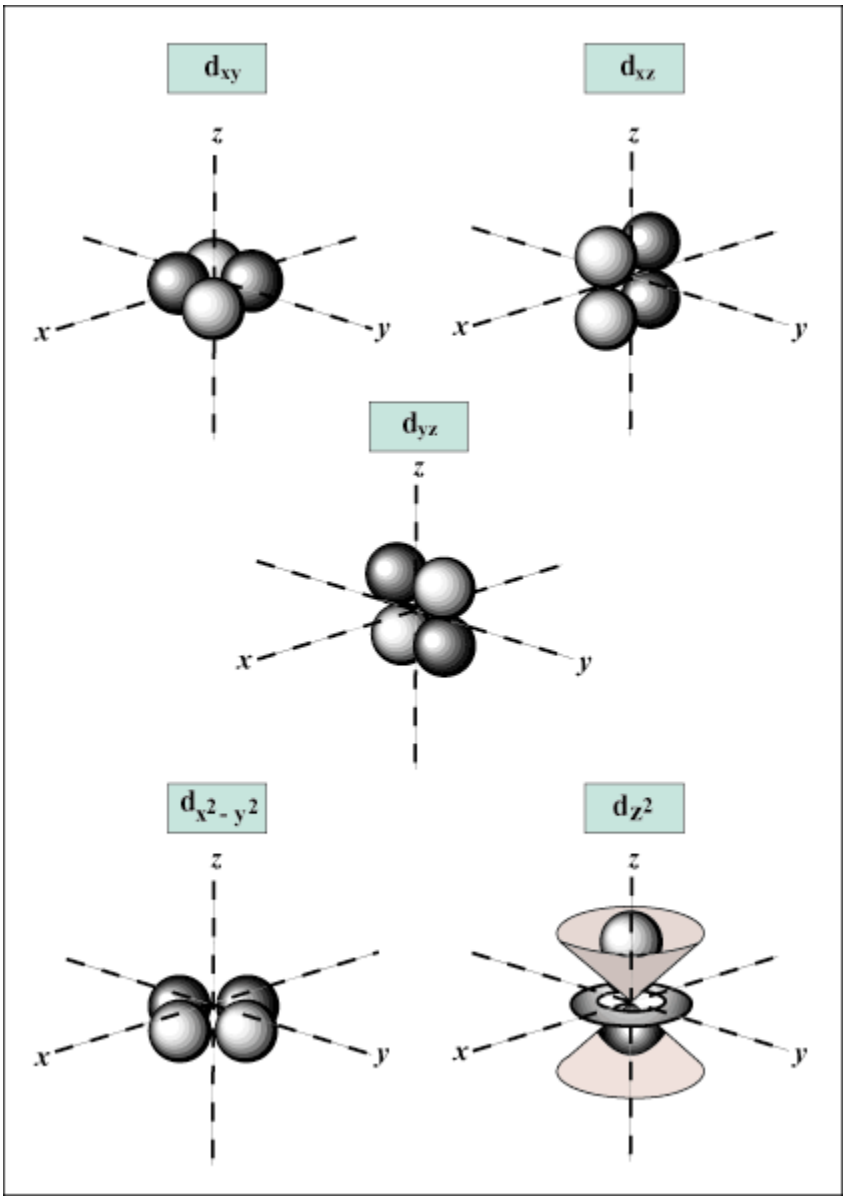


Figure %: d orbitals

Spin Quantum Number (s):

The spin quantum number tells whether a given electron is spin up (+1/2) or spin down (-1/2). An orbital contains two electrons, and each of those electrons must have different spins.

It is often convenient to depict orbitals in an orbital energy diagram, as seen below in . Such diagrams show the orbitals and their electron occupancies, as well as any orbital interactions that exist. In this case we have the orbitals of the hydrogen atom with electrons omitted. The first electron shell (n = 1) contains just the 1s orbital. The second shell (n = 2) holds a 2s orbital and three 2porbitals. The third shell (n = 3) holds one 3s orbital, three 3p orbitals, and five 3d orbitals, and so forth. Note that the relative spacing between orbitals becomes smaller for larger n. In fact, as n gets large the spacing becomes infinitesimally small.

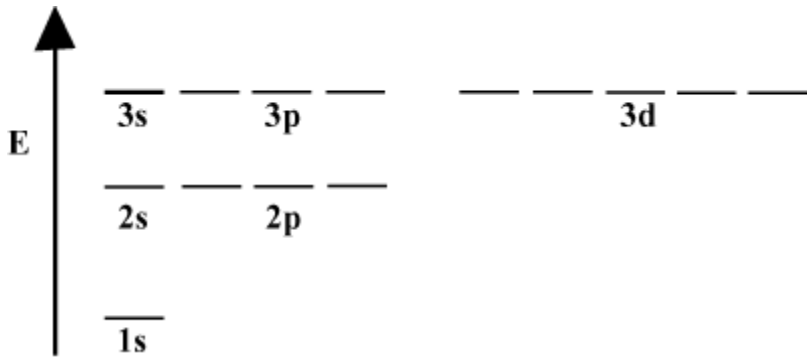


Figure %: Energy diagram of the unoccupied atomic orbitals of hydrogen. Potential energy is on the y-axis.

Multi-Electron Atoms

The electrons in an atom fill up its atomic orbitals according to the Aufbau Principle; "Aufbau," in German, means "building up." The Aufbau Principle, which incorporates the Pauli Exclusion Principle and Hund's Rule prescribes a few simple rules to determine the order in which electrons fill atomic orbitals:

INORGANIC CHEMISTRY

1. Electrons always fill orbitals of lower energy first. 1s is filled before 2s, and 2s before 2p.
2. The Pauli Exclusion Principle states no two electrons within a particular atom can have identical quantum numbers. In function, this principle means that if two electrons occupy the same orbital, they must have opposite spin.
3. Hund's Rule states that when an electron joins an atom and has to choose between two or more orbitals of the same energy, the electron will prefer to enter an empty orbital rather than one already occupied. As more electrons are added to the atom, these electrons tend to half-fill orbitals of the same energy before pairing with existing electrons to fill orbitals.

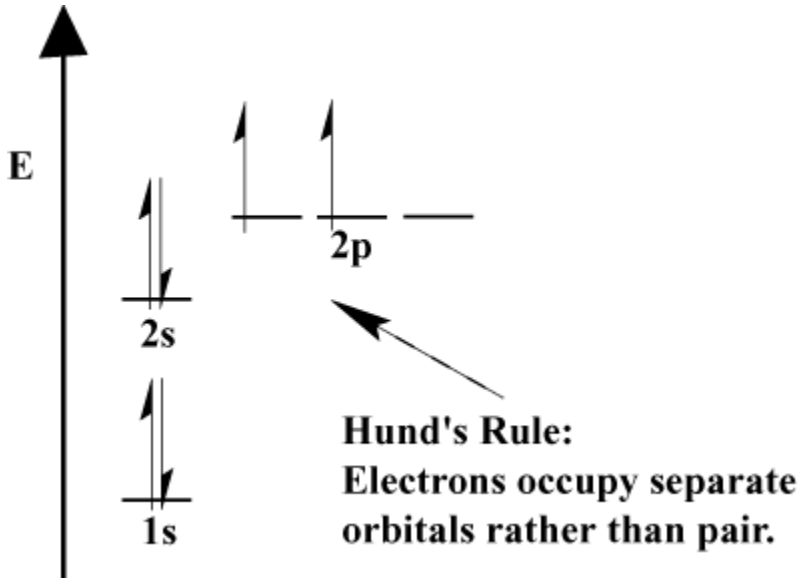


Figure : The ground state electron configuration of carbon, which has a total of six electrons. The configuration is determined by applying the rules of the Aufbau Principle.

INORGANIC CHEMISTRY

The outermost orbital shell of an atom is called its valence shell, and the electrons in the valence shell are valence electrons. Valence electrons are the highest energy electrons in an atom and are therefore the most reactive. While inner electrons (those not in the valence shell) typically don't participate in chemical bonding and reactions, valence electrons can be gained, lost, or shared to form chemical bonds. For this reason, elements with the same number of valence electrons tend to have similar chemical properties, since they tend to gain, lose, or share valence electrons in the same way. The Periodic Table was designed with this feature in mind. Each element has a number of valence electrons equal to its group number on the Periodic Table.

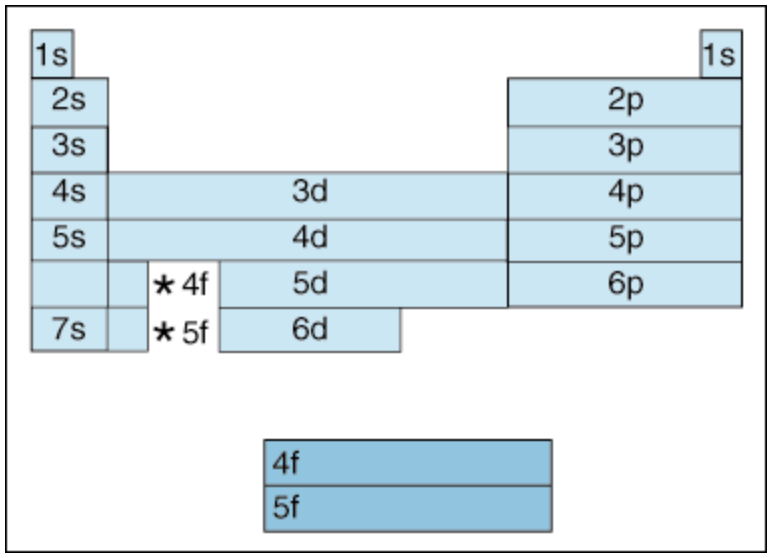


Figure : The periodicity of valence electrons

This table illustrates a number of interesting, and complicating, features of electron configuration.

INORGANIC CHEMISTRY

First, as electrons become higher in energy, a shift takes place. Up until now, we have said that as the principle quantum number, increases, so does the energy level of the orbital. And, as we stated above in the Aufbau principle, electrons fill lower energy orbitals before filling higher energy orbitals. However, the diagram above clearly shows that the 4s orbital is filled before the 3d orbital. In other words, once we get to principle quantum number 3, the highest subshells of the lower quantum numbers eclipse in energy the lowest subshells of higher quantum numbers: 3d is of higher energy than 4s.

Second, the above indicates a method of describing an element according to its electron configuration. As you move from left to right across the periodic table, the above diagram shows the order in which orbitals are filled. If we were the actually break down the above diagram into groups rather than the blocks we have, it would show how exactly how many electrons each element has. For example, the element of hydrogen, located in the uppermost left-hand corner of the periodic table, is described as $1s^1$, with the s describing which orbital contains electrons and the ^{1} describing how many electrons reside in that orbital. Lithium, which resides on the periodic table just below hydrogen, would be described as $1s^22s^1$. The electron configurations of the first ten elements are shown below (note that the valence electrons are the electron in highest energy shell, not just the electrons in the highest energy subshell).

INORGANIC CHEMISTRY

Atomic Number	Element Symbol	Electron Configuration	Number of Valence Electrons
1	H	$1s^1$	1
2	He	$1s^2$	2
3	Li	$1s^2 2s^1$	1
4	Be	$1s^2 2s^2$	2
5	B	$1s^2 2s^2 2p^1$	3
6	C	$1s^2 2s^2 2p^2$	4
7	N	$1s^2 2s^2 2p^3$	5
8	O	$1s^2 2s^2 2p^4$	6
9	F	$1s^2 2s^2 2p^5$	7
10	Ne	$1s^2 2s^2 2p^6$	8

The Octet Rule

Our discussion of valence electron configurations leads us to one of the cardinal tenets of chemical bonding, the octet rule. The octet rule states that atoms become especially stable when their valence shells gain a full complement of valence electrons. For example, in above, Helium (He) and Neon (Ne) have outer valence shells that are completely filled, so neither has a tendency to gain or lose electrons. Therefore, Helium and Neon, two of the so-called Noble gases, exist in free atomic form and do not usually form chemical bonds with other atoms.

Most elements, however, do not have a full outer shell and are too unstable to exist as free atoms. Instead they seek to fill their outer electron shells by forming chemical bonds with other atoms and thereby attain Noble Gas configuration. An element will tend to take the shortest path to achieving Noble Gas configuration, whether that means gaining or losing one electron. For example, sodium (Na), which has a single electron in its outer 3s orbital, can lose that electron to attain the electron configuration of neon. Chlorine, with seven valence electrons, can gain one electron

to attain the configuration of argon. When two different elements have the same electron configuration, they are called isoelectronic.

The electron configuration of an atom also has consequences on its behavior in relation to magnetic fields. Such behavior is dependent on the number of electrons an atom has that are spin paired. Remember that Hund's Rule and the Pauli Exclusion Principle combine to dictate that an atom's orbitals will all half-fill before beginning to completely fill, and that when they completely fill with two electrons, those two electrons will have opposite spins.