**Electronic structure of Atoms**

**An Introduction to Electronic distribution .**

All matter is composed of atoms . By the end of the nineteenth century , scientists were convinced that matter was composed of atoms .

The atom was identified as the smallest representative sample of an element .

How ever , an English physicist named J.J.Thomson (1856-1940 ) complicated the picture by discovering an even smaller and more fundamental particle called the electron .

Thomson discover that electrons are negatively charge , that they are much smaller and lighter than atoms .

The discovery of negative charged particles within atoms raised the question of a balancing positive charge .

Atoms were know to be charge-neutral , so they must contain positive charge that balanced the negative charge of electrons.

In 1909 Rutherford (1871-1937) , who had worked under Thomson , proposed the nuclear theory of the atom which has three parts :

1-Most of the atom's mast and all of its positive charge are contained in a small core called the nucleus .

2-Most of the volume of the atom is empty space through which the tiny , negatively charged electrons are dispersed .

3-There are as many negatively charged electron outside the nucleus as there are positively charged particles

(proton ) inside the nucleus , so that the atom in electrically neutral .

Later work by Rutherford and others demonstrated that the atom's nucleus contains both positively charged protons and neutral particles called neutrons .The dense nucleus makes up more than 99.9% of the mass of the atom , but occupies only a small fraction of its volume . The electrons are distributed through a much large region , but don't have much mass.

The properties of protons , neutrons and electrons .

Protons and neutrons have very similar masses , the mass of the proton is 1.6762 x 10-27 kg,

And the mass of neutron is a close 1.67493 x 10-27kg .

A more common unit to express these masses , however , is the ''atomic mass unit(amu)'' defined as one – twelfth of the mass of carbon atom containing six protons and six neutrons .

In this unit , a proton has a mass of 1.0073 amu and a neutron has a mass of 1.0087 amu .

Electrons , by contrast , have an almost negligible mass of 0.00091 x 10-27 kg or approximately 0.00055 amu .

The proton and the electron both have electrical charge . the proton's charge is 1+ and the electron's charge 1- .

The charge of the proton and the electron are equal in magnitude but opposite in sign , so that when the two particles are paired , the charge exactly cancel .

The neutron has no charge .

Q/ An atom with which of these compositions would have a mass of approximately 12 amu and be charge neutral ?

a)6 protons and 6 electrons .

b)3 protons , 3 neutrons and 6 electrons .

c)6 protons , 6 neutrons and 6 electrons .

d)12 neutrons and 12 electrons .

we have seen that atoms are composed of protons, neutrons and electrons . However , it is the number of protons in the nucleus of an atoms that identifies it as a particular element . for example , atoms with 2 protons in their nucleus are helium atoms , atoms with 13 protons in their nucleus are aluminum atoms , and atoms with 92 protons in their nucleus are uranium atoms .

The number of protons in an atom's nucleus defines the element .

The number of protons in the nucleus of an atom is called ''atomic number '' and is given the symbol Z.

Atoms with the same number of protons but different number of neutrons are called ''isotopes'' , for example , all neon atoms in nature contain 10 protons , but they may have 10,11 or 12 neutrons .

Some elements , such as beryllium (Be) and aluminum (Al) , have only one naturally occurring isotope .

The sum of the number of protons and neutrons in an atom called the " mass number " and in given the symbol A . { A =number of protons + number of neutrons }

Table {1- 1} Neon isotopes.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Percent Natural Abundance | Mass number [A] | Number of Neutrons | Number of protons | 5ymbol |
| 90.48%  0.27%  9.25% | 20  21  22 | 10  11  12 | 10  10  10 | 20  Ne- 20or 10 Ne  21  Ne -21 or 10 Ne  22  Ne – 22 or 10 Ne |

Isotopes are often symbolized in the following way :-

Mass number → A

X ← chemical symbol

Atomic number→ Z

Electron configurations :How Electrons occupy orbitals

An electron configuration simply shows the occupation of orbitals by electrons for particular atom . For example , the electron configuration for a ground state hydrogen atom is :-

H = 1S1← number of electron in orbital .

orbital↑

The electron configuration tells us that hydrogen's single electron is in the 1S orbital.

Another way the represent this information is with an orbital diagram , Which , given similar information but shows the electrons as arrows in a box representing the orbital

The orbital diagram for a ground – state hydrogen atom is :

H

↑

1S

The box represents the 1S orbital and the arrow within the box represents the electron in the 1S orbital .

In orbital diagrams , the direction of the arrow (pointing up or down ) represents electron spin , a fundamental properties of electrons .All electrons have spin . The pauli exclusion principle state the orbitals may hold no more than two electrons with opposite , spins . we symbolize this as two arrows pointing in opposite directions ↑↓ .

Helium atom , for example have two electrons . The electron configuration and orbital diagram are :-

Electron configuration orbital diagram

↑↓

He 1S2

1S

Since we know that electrons occupy the lowest – energy orbitals available , and since we know that only two electrons (with opposing spins ) are allowed in each orbital, we can continue to build ground – state electron configurations for the rest of the elements as long as we know the energy ordering of the orbitals .

Notice that , for multi –electron atoms, the subshells with in a principal shell do not have the same energy. Thus in elements other than hydrogen, the energy ordering is not determined by the principal quantum number alone, for example, the 4S subshell is lower in energy than the 3d subshell, even though its principal quantum number is higher. Using this relative energy ordering , we can write ground-state electron configurations and orbital diagrams for other elements for lithium, which has three electrons , the electron configuration and orbitaldiagram are:

Electron configuration Orbital diagram

Li 1S2 2S1

↑↓

↑

1S 2S

For carbon, which has six electrons.

Electron configuration Orbital digram

C 1S2  2S2 2P2

↑↓

↑↓

↑

↑

1S 2S 2P

Energy

4d 4d 4d 4d 4d

5S

4P 4P 4P

3d 3d 3d 3d 3d

4S

3P 3P 3P

3S

2P 2P 2P

2S

1S

Figure (1-1) Energy ordering of orbitals for multi – electron atoms

Notice that the 2p electrons occupy the p orbitals [ of egual energy] singly , rather than paining in one orbital. This is a result of Hund,s rule , which states that when filling orbitals of equal energy , electrons fill them singly first , with parallel spins.

Summarize what we have learned so far:

1- Electrons occupy orbitals so as to minimize the energy of the atom, therefore lower energy orbitals fill before higher energy orbitals , Orbitals fill in the following order:

1S 2S 2P 3S 3P 4S 3d 4P 5S 4d 5P 6S { Figure 1- 2 }.

2- Orbitals can hold no more than two electrons each . When two electrons occupy the same orbital , they must have opposing spins . This is known as the Pauli exclusion principle . 3- When orbitals of identical energy are available , these are first occupied single with parallel spins rather than in pairs , This is known as Hund's rule.

1S

2S 2P

3S 3P 3d

4S 4P 4d 4f

5S 5P 5d 5f

6S 6P 6d

7S Figure {1 - 2} Orbital filling order .

Consider the electron configurations and orbital diagrams for elements with atomic numbers 3 through 10 .

Symboi {# e } Electron configuration Orbital diagram

Li {3} 1S2 2S1

↑

↑↓

1S 2S

↑↓

↑↓

Be {4} 1S2 2S2

1S 2S

B {5} 1S2 2S2 2P1

↓↑

↓↑

↑

1S 2S 2P

C {6}1S2 2S2 2P2

↑

↑

↓↑

↓↑

1S 2S 2P

↑

↑

↑

↓↑

↓↑

N {7} 1S2 2S2 2P3

1S 2S 2P

↑

↑

↓↑

↓↑

↓↑

O {8} 1S2 2S2 2P4

1S 2S 2P

F {9} 1S2 2S2 2P5

↑

↓↑

↓↑

↓↑

↓↑

2P 1S 2S

Ne {10} 1S2 2S2 2P6

↓↑

↓↑

↓↑

↓↑

↓↑

1S 2S 2P

The electron configuration of neon (Ne) represent the complete filling of the n=2 principal shell . When writing electron configurations for elements beyond (Ne) or beyond any ather noble gas – the electron configuration of the previous noble gas in often abbreviated by the symbol for the noble gas in brackets . for example :-

Na 1S2 2S2 2P6 3S1

This can also be written as

Na [Ne]3S1 .

Noble gas : He (2) , Ne (10) , Ar (18) , Kr(36) , Xe (54) , Rn(86).

Q) Write electron configurations for each of the fallowing elements :-

a)Mg b)S c)Ga d)Si

Q)Which of the following pairs of elements have the same total number of electrons in p orbitals :-

a)Na and K b)K and Kr c)P and N d)Ar and Ca .

Valence electrons :- The electrons in the outer most principal shell , these electrons are important because they are involved in chemical bonding .

Core electrons :- Electrons that are not in the outermost principal shell .

Si 1S2  2S2 2P 6  3S2 3P2 \_\_\_\_\_\_\_\_\_\_\_\_\_\_ \_\_\_\_\_\_\_\_\_\_\_\_

↑ ↑

Core electrons valence electrons .

Q)Write an electron configuration for selenium (Se) and identify the valence electrons and the core electrons .

The periodic table can be divided into blocks representing the filling of particular sub shells :-

1-The first two columns on the left side of the periodic table are the S block with outer electron configuration of ns1(first column ) and ns2 (second column ) .

2-The six columns on the right side of the periodic table are the p block with outer electron configurations of

Ns2 np1,ns2np2,ns2np3,ns2np4,ns2np5 (halogens ), ns2np6 (nobles gases ).

3-The transition metals are the d block .

4-The lanthanides and actinides are the f block .

Notice :-

1-Except helium , the number of valence electrons for any main –group element in equal to the group number of its column . For example , chlorine has (7) valence electrons because it is the colume with group (7A).

2-The row number in the periodic table in equal to the number of the highest principal shell (n value ).

For example , since chlorine is in row 3, its highest principal shell in the n = 3 shell .

3- The transition metals have electron configuration with trends that differ some what from main – group element.

As you move across a row in the d block , the d orbitals are filling figure (1-3) .

However , the principal quantum number of the d orbital being filled across each row in the transition series is equal to the raw number minus one (in the fourth row , the 3d orbitals fill , in the fifth row , the 4d orbitals fill , and so on ). For the first transition series , the outer configuration is 4S2 3dx (x=number of d electrons ) with two exceptions Cr is 4S1 3d5 and Cu is 4s1 3d10

Electron configurations of the first transition series elements :-

Element Electron configurations

3d 4S

↑

↓↑

Sc [Ar] 4S2 3d1

4S 3d

↑

↓↑

↑

Ti [Ar ] 4S2 3d 2

4S 3d

↑

↑

↑

↓↑

V [Ar ] 4S2 3d 3

4S 3d

[Ar ] 4S1 3d 5  Cr

↑

↑

↑

↑

↑

↓↑

4S 3d

↑

↑

↑

↑

↑

↓↑

Mn [Ar ] 4S2 3d 5

4S 3d

↑

↑

↑

↑

↓↑

↓↑

Fe [Ar ] 4S2 3d6

3d 4S

↑

↑

↑

↓↑

↓↑

↓↑

Co [Ar ] 4S2 3d 7

4S 3d

↑

↑

↓↑

↓↑

↓↑

↓↑

Ni [Ar ] 4S2 3d 8

4S 3d

Cu [Ar ] 4S1 3d 10

↓↑

↓↑

↓↑

↓↑

↓↑

↓↑

4S 3d

Zn [Ar ] 4S2 3d 10

↓↑

↓↑

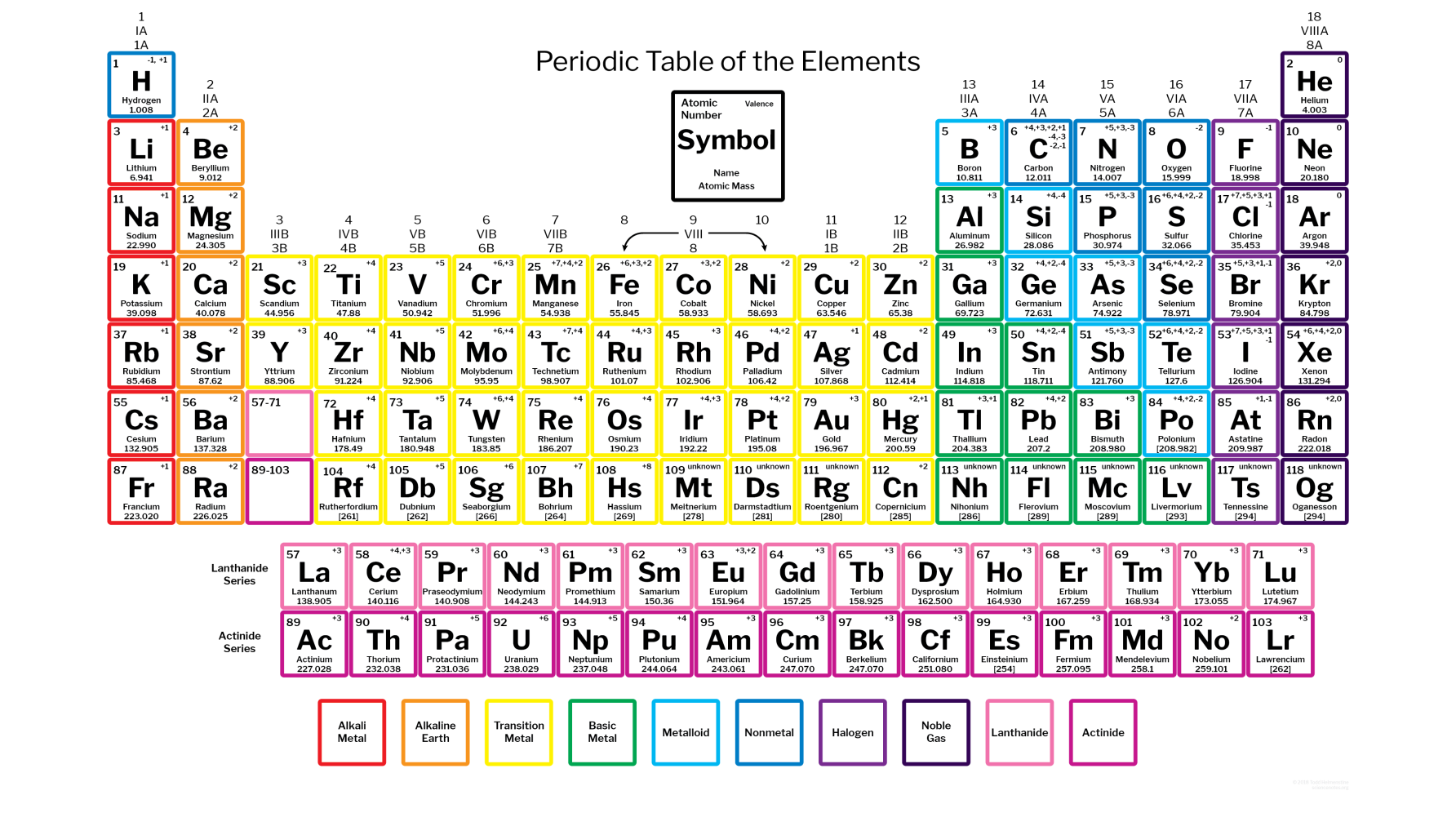
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↓↑

↓↑

Figure (1-3)



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