

## Atomic Structure

### Topics:-

1. Introduction
2. Fundamental particles
3. Atomic Number and Mass Number
4. Isotopes, Isobars and Isotones
5. Atomic Models → Rutherford's Atomic Model  
→ Bohr's Atomic Model
6. Orbita and Orbitals
7. Quantum Numbers
8. Aufbau Principle
9. Electronic Configurations.

## 1. Introduction

Atom: Atom is the smallest part of a molecule which consists of three fundamental particles. Such as: Electron, Proton and neutron

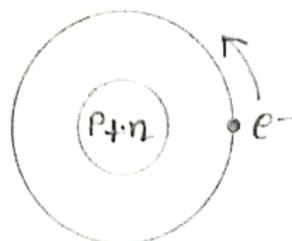


Fig: Atom

2. Fundamental Particles: The description of three fundamental particles: Electron, proton and neutron are stated below:

Electron: Electron was discovered in 1897 by Sir J.J. Thomson. It has a mass of  $9.1085 \times 10^{-31}$  gm or  $9.1085 \times 10^{-31}$  kg. It carries a negative charge of the quantity  $1.6 \times 10^{-19}$  C. It is positioned at outer nucleus and is denoted by ' $e^-$ '.

Proton: Proton was discovered in 1919 by Rutherford. It carries the weight of  $1.673 \times 10^{-24}$  gm. It has a positive charge of  $1.6 \times 10^{-19}$  C. It is positioned at Nucleus and is denoted by ' $p$ '.

Neutron: Neutron was discovered by Chadwick in 1932. It has a mass of  $1.675 \times 10^{-24}$  gm. It has no charge. It is positioned at Nucleus and is denoted by ' $n$ '.

short technique to remember the characteristics of fundamental particles:

Characteristics	Electron	Proton	Neutron
Invented in	1897	1919	1932
Invented by	Sir J.J. Thomson	Rutherford	Chadwick
Mass	$9.1085 \times 10^{-31} \text{ kg}$ $9.1085 \times 10^{-28} \text{ gm}$	$1.673 \times 10^{-24} \text{ gm}$	$1.675 \times 10^{-24} \text{ gm}$
charge	$-1.6 \times 10^{-19} \text{ C}$	$1.6 \times 10^{-19} \text{ C}$	Neutral
Position	Outer Nucleus	Nucleus	Nucleus
Denoted by	'e <sup>-</sup> '	'p'	'n'

### 3. Atomic Number and Mass Number:

(I) Atomic Number:- The number of protons that present in a nucleus of an atom is called Atomic number. It is denoted by 'Z'.

Atomic number = number of protons

$$Z = 'p'$$

If it's neutral then,  $Z = 'p' = 'e^-'$

(II) Atomic Mass Number: The sum of number of protons and neutrons that present in a nucleus of an atom is called Mass number.

Atomic mass number = number of protons + number of neutrons  
Therefore,  $A = p+n$

(III) Rule for writing atomic no, mass no, charge and no of atoms:-

Symbol of atom :-

$A \times$  (mt) number of charges  
 $n \rightarrow$  number of atoms

#### 4. Isotopes, Isobars and Isotones:

(I) Isotopes: The atoms which have same atomic / proton number but different mass and neutron number are called Isotopes of each other.

Example: 1.  $^1_1\text{H}$ ,  $^2_1\text{H}$ ,  $^3_1\text{H}$   
Protium Duterium Tritium

2.  $^{12}_6\text{C}$ ,  $^{13}_6\text{C}$ ,  $^{14}_6\text{C}$       3.  $^{16}_8\text{O}$ ,  $^{17}_8\text{O}$ ,  $^{18}_8\text{O}$

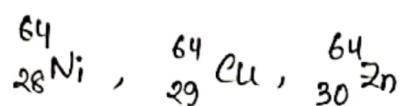
Carbon-12, Carbon-13, Carbon-14      Oxygen-16      Oxygen-17      Oxygen-18

Q) Comment on -the physical and chemical properties of Isotopes.

⇒ They have similar chemical properties because isotopes of an element have the same number of electrons as an atom of that element. The electron arrangement is the same owing to same chemical properties. However they have different numbers of neutrons, which affects the mass number. Mass number determines the physical properties such as boiling, melting, density etc. That's why, we can say that due to difference in atomic mass and mass number the physical properties of Isotopes of the same element are not identical.

(II) Isobars: The atoms which have same mass number but different protons and neutron numbers are called Isobars of each other.

Example:



Comment on the physical and chemical properties of Isobars:

→ Isobars always have different atomic structure because of the difference in atomic numbers. Therefore they are always different chemical elements. Thus, isobar has different chemical properties.

By now we know that atomic mass determines the physical properties and atomic masses in isobars are same. Therefore they have similar physical properties.

(III) Isotones: The atoms which have different proton and mass numbers but same neutron number, are called Isotones of each other.

Example:  $^{30}_{14}\text{Si}, ^{31}_{15}\text{P}, ^{32}_{16}\text{S}$

Comment on the physical and chemical properties of Isotones:

→ The chemical properties of isotones of an element are different because the electron arrangement is different. The physical properties of Isotones are also different due to having different mass numbers.

5. Atomic Models:- After the discovery of electrons the realization was that atoms are divisible. Different scientists forwarded different concepts about the structure of atom in the period of 1897- 1932. These concepts are known as atomic models.

The atomic models are:-

1. Thomson atom model (1898)
2. Rutherford atom model (1911)
3. Bohr atom model (1913)
4. Bohr-Sommerfeld atom fine model (1916)
5. Wave-mechanical atom model (1924) → Dual nature of electron  
(a) Particle (b) Wave

Rutherford's Atom Model: Based on  $\alpha$ - particle scattering experiment, Rutherford forwarded his atom model. The main postulates of Rutherford atom model are as follows:

1. An atom has two parts: (i) Nucleus and (ii) extra nuclear part. Nucleus is a massive positively charged body at the centre of the atom.
2. Atom is electrically neutral. so a number of electrons equal to positive charges of the nucleus are present in an atom. Electrons are in constant motion around the nucleus in different orbits like the planets in a solar system.
3. Due to constant motion of the electrons around the nucleus, the outward centrifugal force is exactly

counter balanced by the inward electrostatic attraction between the electrons and nucleus.

### Limitations:

1. Rutherford's model failed to explain the stability of atoms.
2. This model cannot give any explanation of the atomic spectra.
3. Rutherford did not give any idea about the shape and size of the orbits of electrons in an atom.
4. There were no explanation about the rotation of many electrons in an orbit.

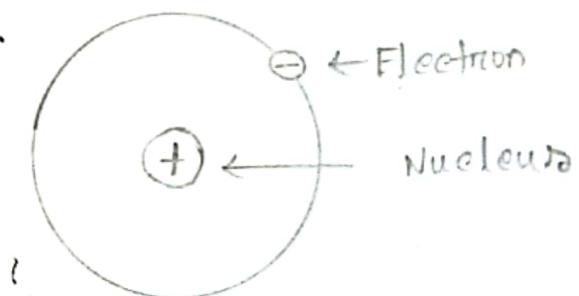


Fig: Rutherford Atom Model

### Bohr Atom Model:

In 1913, Niels Bohr proposed his famous atom model, which not only described the structure of atom, but also gave an explanation about the origin of atomic spectra.

The postulates of Bohr Atom Model are as follows:

1. According to Bohr, electrons can rotate in definite circular paths around the nucleus. These circular paths are known as stationary orbits or energy levels of electrons. Each energy level has a definite or fixed energy.

2. The permissible orbits or energy levels are for those which angular momentum of the revolving electrons are an integral multiple of  $\frac{h}{2\pi}$ . The angular momentum,  $mv\pi = n \times \frac{h}{2\pi}$ .
3. An electron can jump from an orbit to another. When electron jumps from higher energy level to lower energy level, then it emits energy. On the other hand, if an electron jumps from lower to higher energy level then it absorbs energy.

#### Limitations:

- It violates the Heisenberg Uncertainty principle.
- It failed to explain the Zeeman effect when the spectral line is split into several components in the presence of a magnetic field.
- It failed to explain the Stark effect when the spectral line gets split up into fine lines in the presence of an electric field.

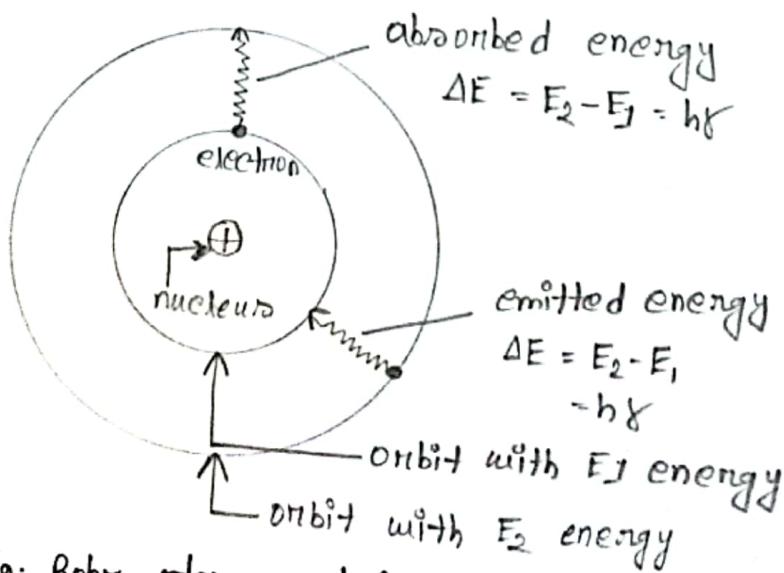


Fig: Bohr atom model

## 6. Orbita and orbitals:

1. Orbit: According to Bohr Atom model, there are some fixed circular paths for electrons to revolve around the nucleus. These fixed circular paths are known as orbits. The orbits are characterized by values of principal quantum number. The orbits nearest to the nucleus is the 1st orbit and for it  $n=1$ . Similarly the next orbits are known as 2nd, 3rd and 4th orbits and for them  $n=2, 3, 4$  etc. They are gradually more apart from the nucleus and hence their sizes increase gradually in this order.

2. Orbital: An atomic orbital is defined as the region around the nucleus in which the probability of finding the electron cloud is maximum. The electron cloud being denser in some regions and less dense in some other regions, the probability of finding an electron cloud decreases with distance, but does not become zero.

## Difference between orbit and orbital:

Orbit	Orbital
1. The word 'orbit' originates from Bohr atom model. According to this model, electrons revolve around nucleus in definite circular paths. These paths are called orbit.	1. The word 'Orbital' originates from quantum mechanics. The regions around the nucleus, where the probability of finding electrons is high (about 90%) are known as orbital.
2. The orbits are circular.	2. The shapes of different orbitals are different. Example: S orbitals are spherical, P orbitals are dumbbell shaped with two lobes. d orbitals are double dumbbell shaped with four lobes.
3. Orbita are related to Principal quantum number, n.	3. Orbitals are related to three quantum numbers n, l and m.
4. Orbita are designated by the letters K, L, M, N, O etc.	4. When $l=0, 1, 2, 3$ etc. the orbitals are designated s, p, d, f etc.
5. Each orbit can accommodate maximum $2n^2$ electrons.	5. Each orbital can accommodate maximum 2 electrons with opposite spin

## 7. Quantum Numbers:

According to quantum mechanics, three interrelated numbers are required to express the size, shape and orientation of the orbitals of electrons in an atom. Moreover, there is a number to express the direction of spin of the electron. These four correlated numbers are called quantum numbers which are as follows:

1. Principal quantum number,  $n$
2. Azimuthal quantum number,  $l$
3. Magnetic quantum number,  $m$
4. Spin quantum number,  $s$ .

1. Principal quantum number: The quantum number that expresses the main energy level in which the electrons are moving around the nucleus is the principal quantum number. It is expressed by  $n$ .

Where,  $n = 1 = 1\text{st orbit} = \text{K shell} = 2n^2 = 2(1)^2 = 2$   
 $n = 2 = 2\text{nd orbit} = \text{L shell} = 2n^2 = 2(2)^2 = 8$   
 $n = 3 = 3\text{rd orbit} = \text{M shell} = 2n^2 = 2(3)^2 = 18$   
 $n = 4 = 4\text{th shell} = \text{N shell} = 2n^2 = 2(4)^2 = 32$   
 $n = 5 = 5\text{th shell} = \text{O shell} = 2n^2 = 2(5)^2 = 50$   
 $n = 6 = 6\text{th shell} = \text{P shell} = 2n^2 = 2(6)^2 = 72$

The maximum number of electrons which can occupy in each particular orbit is given by  $2n^2$ .

2. Secondary quantum number: The quantum number which is used to indicate subshells is known as subsidiary quantum number. It is denoted by ' $l$ '. It may have values from 0 to  $(n-1)$ . The value of ' $l$ ' determines the shape of the orbitals. When  $l=0 \rightarrow$  s orbital  
 $l=1 \rightarrow$  p orbital  
 $l=2 \rightarrow$  d orbital  
 $l=3 \rightarrow$  f orbital

For 1st shell,  $n=1, l=0, (1s)$

2nd shell,  $n=2, l=0, 1 (2s, 2p)$

3rd shell,  $n=3, l=0, 1, 2 (3s, 3p, 3d)$

4th shell,  $n=4, l=0, 1, 2, 3 (4s, 4p, 4d, 4f)$

The maximum capacity of an orbital to hold electrons is  $2 \times (2l+1)$ .

3. Magnetic quantum number: The magnetic quantum number defines the orientation of a given orbital in space. It is denoted by ' $m$ '. It may have values from -1 to +1, including 0. So, there may be  $(2l+1)$  values of ' $m$ ' for each value of ' $l$ '. Its value gives the total number of orbital present in each orbit.

For s subshell,  $l=0$  then  $m=0$

$\therefore$  in s subshell exists 1 orbital.

For p subshell,  $l=1$  then  $m=+1, 0, -1$

$\therefore$  in p subshell exists 3 orbital

For d subshell,  $l=2$  then  $m=+2, +1, 0, -1, -2$

$\therefore$  in d subshell exists 5 orbital

For f subshell,  $l=3$  then  $m = 3, 2, 1, 0, -1, -2, -3$ .  
in f subshell exists 7 orbitals.

4. Spin quantum numbers: While rotating around the nucleus the electrons also rotate around its own axis either in clockwise or in anticlockwise direction. Spin quantum number is used to describe this. It is expressed by  $s$  and its value is  $+\frac{1}{2}$  when clockwise and its value is  $-\frac{1}{2}$  when anticlockwise. This is also denoted by arrows pointing up and down. i.e.  $\uparrow$  and  $\downarrow$  respectively.

8. Aufbau principle: In an atom, the electrons occupy different orbitals according to their increasing energy levels. That means, electrons first occupy the orbital of lowest energy and systematically then the orbitals of higher energy level. This rule is called Aufbau Principle.  
Determination of order of orbitals:

To determine the comparative energy of different orbitals the following two rules are generally used:  
Rule-1:-

among several orbitals, the orbital whose  $(n+l)$  value is less, will be of lower energy.

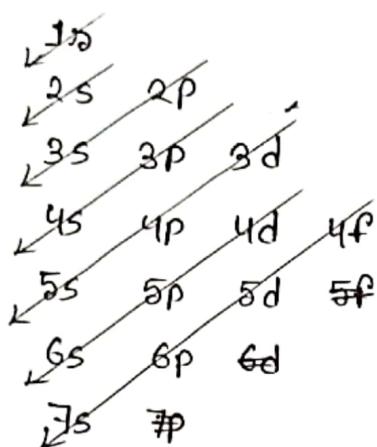
Rule-2:-

If two or more orbitals possess same value of  $(n+l)$  then the orbital whose value of ' $n$ ' is less will be of lower energy.

The orbital of different energy from lower to higher gradually are as follows:

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

Order of energy level of different orbitals:



9. Electronic Configurations: The electronic configuration of an element describes how electrons are distributed in its atomic orbitals.

Electronic configuration is written by following the three principles:-

1. Aufbau Principle
2. Pauli Exclusion Principle
3. Hund's Rule

1. Aufbau Principle: The aufbau principle dictates that electrons will occupy the orbitals having lower energies before occupying higher energy orbitals.

2. Pauli Exclusion Principle: The pauli Exclusion Principle states that a maximum of two electrons, each having

Opposite spins, can fit in an orbital.

3. Hund's Rule: It states that every orbital in a given subshell is singly occupied by electrons before a second electron is filled in an orbital.

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

There are three 2p orbitals of same energy which are  $p_x, p_y, p_z$ .

$N(7) = \begin{array}{c} 1s^2 \\ \boxed{\uparrow\downarrow} \end{array} \begin{array}{c} 2s^2 \\ \boxed{\uparrow\downarrow} \end{array} \begin{array}{c} 2p^3 \\ \boxed{\uparrow\uparrow\uparrow} \end{array}$

Deviation of Electronic Configuration from the General Rule:

The electronic configuration of almost all elements can be confirmed according to Aufbau principle.

But there are some deviations. Two major reasons behind these deviations are as follows:

① More stability of half-filled and full-filled orbitals:

It is found that the degenerate orbitals gain more stability, when they are exactly half-filled or full-filled.

That means that  $np^3, np^6, nd^5, nd^{10}, nf^7, nf^{14}$ .

Configurations are more stable. For this reason, the configuration  $(n-1)d^5 ns^1$  becomes more stable than  $(n-1)d^4 ns^2$ .

Q) Why  $1p$  /  $1d$  /  $2f$  /  $2d$  /  $3f$  is not possible?

We know that,  $l=0 = s$

$l=1 = p$

$l=2 = d$

$l=3 = f$

For  $1p$ ,

Hence,  $n=1$ ,  $l=0$

but for  $p$  orbital,  $l=1$

Since,  $n=1$ ,  $l=1$  is not possible;

Hence,  $1p$  is not possible.

For  $1d$ ,

Hence,  $n=1$ ,  $l=0$

but for  $d$  orbital  $l=2$

Since,  $n=1$ ,  $l=2$  is not possible.

Hence,  $1d$  is not possible.

For  $1f$ ,

Hence,  $n=1$ ,  $l=0$

but for  $f$  orbital  $l=3$

Since,  $n=1$ ,  $l=3$  is not possible.

Hence,  $1f$  is not possible.

For  $2d$ ,

Hence,  $n=2$ ,  $l=0, 1$

but for  $d$  orbital  $l=2$

Since,  $n=2$ ,  $l=2$  is not possible.

Hence,  $2d$  is not possible.

For  $2f$ ,

Hence,  $n=2$ ,  $l=0, 1$

but for  $f$  orbital  $l=3$

Since,  $n=2$ ,  $l=3$  is not possible.

Hence,  $2f$  is not possible.

For 3f,

Hence,  $n = 3$ ,  $l = 0, 1, 2$

But for  $n$ , f orbital  $l = 3$

Since,  $n = 3$ ,  $l = 3$  is not possible.

Hence, 3f is not possible.

Q Which sets of following quantum numbers are allowable or not? If not give the proper reasons.

①  $n = 2, l = 1, m = 0, s = +\frac{1}{2}$  (Allowable)

②  $n = 3, l = 3, m = +2, s = -\frac{1}{2}$  (Not allowable)  $\Rightarrow (n = 3 \neq l = 3) (l = 0, 1, 2)$

③  $n = 1, l = 0, m = +1, s = +\frac{1}{2}$  (Not allowable)  $\Rightarrow (n = 1, m = +1 \text{ is not possible})$

④  $n = 4, l = 3, m = -3, s = -\frac{1}{2}$  (Allowable)

Q Suppose an electron is in N shell / 4th orbit / 4f.

Find out the probable four quantum number values for it.

N shell / 4th orbit:

$n = 4$

$l =$	0	1	2	3
$m =$	0	+1 0 -1	+2 0 -1 -2	+3 0 -1 -2 -3
$s =$	$\pm \frac{1}{2}$	$\pm \frac{1}{2}$	$\pm \frac{1}{2}$	$\pm \frac{1}{2}$

Now, for 4f,

$$n=4,$$

for f orbital  $l=3$

$m_l =$	+3	+2	+1	0	-1	-2	-3
$s =$	$\pm \frac{1}{2}$						

- Average the following orbitals according to higher or lower energy.

3d 4s 5p 6s 4f 6p 7s

Solution: 3d 4s 5p 6s 4f 6p 7s

$$3d \rightarrow (n+l) \rightarrow (3+2) = 5$$

$$4s \rightarrow (n+l) \rightarrow (4+0) = 4$$

$$5p \rightarrow (n+l) \rightarrow (5+1) = 6$$

$$6s \rightarrow (n+l) \rightarrow (6+0) = 6$$

$$4f \rightarrow (n+l) \rightarrow (4+3) = 7$$

$$6p \rightarrow (n+l) \rightarrow (6+1) = 7$$

$$7s \rightarrow (n+l) \rightarrow (7+0) = 7$$

$$\therefore 7s > 6p > 4f > 6s > 5p > 3d > 4s$$

$$\therefore 4s < 3d < 5p < 6s < 4f < 6p < 7s.$$

Q) Why are electronic configurations important?

Electronic configurations provide insight into the chemical behaviour of elements by helping determine the valence electrons of an atom. It also helps classify elements into different blocks. This makes it easier to collectively study the properties of the elements.

Q) List the electron configurations of all the noble gases.

The electronic configurations of the noble gases are listed below:

Helium (He)  $\rightarrow 1s^2$

Neon (Ne)  $\rightarrow [He] 2s^2 2p^6$

Argon (Ar)  $\rightarrow [Ne] 3s^2 3p^6$

Krypton (Kr)  $\rightarrow [Ar] 3d^{10} 4s^2 4p^6$

Xenon (Xe)  $\rightarrow [Kr] 4d^{10} 5s^2 5p^6$

Radon (Rn)  $\rightarrow [Xe] 4f^{14} 5d^{10} 6s^2 6p^6$

Q) Why the electronic configuration of Cr(24) and Cu(29) is different?

According to Aufbau principle, the electronic configuration of Cr(24) and Cu(29) is supposed to be:-

Cr(24)  $\rightarrow 1s^2 2s^2 2p^6 3s^2 3p^6 3d^4 4s^2 3d^4$

Cu(29)  $\rightarrow 1s^2 2s^2 2p^6 3s^2 3p^6 \underline{3d^9} 4s^2 3d^9$

But the correct configuration is:-

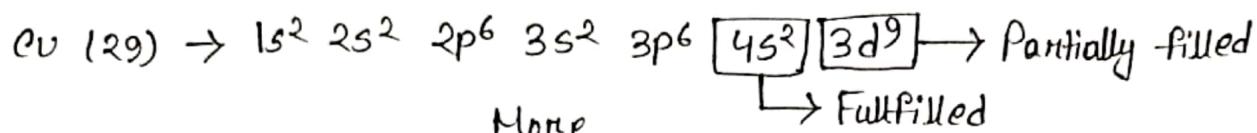
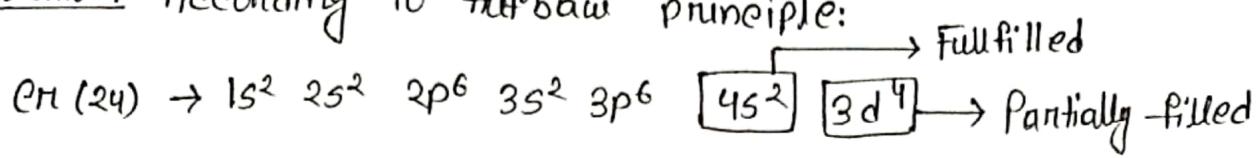
Cr(24)  $\rightarrow 1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1 3d^5$

Cu(29)  $\rightarrow 1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1 3d^{10}$

If we know, the full-filled and half-filled orbitals are more stable than partially filled orbitals. That's why, the electronic configuration of Cr(24) and Cu(29) is different.

Q) Discuss the electronic configuration of Cr(24) and Cu(29)

Solution: According to Aufbau principle:



Fullfilled. Fullfilled

Half-filled. Fullfilled

Half-filled. Half-filled

More stable

Fullfilled. Partially filled

Half-filled. Partially filled

Orbital	Fullfilled	Half-filled	Partially-filled
s	2	1	-
p	6	3	1, 2, 4, 5
d	10	5	1, 2, 3, 4, 5, 7, 8, 9
f	14	7	1, 2, 3, 4, 5, 6, 8, 9, 10, 11, 12, 13

For this reason the configuration  $(n-1)d^5 ns^1$  becomes more stable than  $(n-1)d^4 ns^2$  and  $(n-1)d^{10} ns^1$  becomes more stable than  $(n-1)d^9 ns^2$ .

Therefore the electronic configuration of Cr(24) and Cu(29) are as follows:

