ELECTRONIC STRUCTURE OF ATOMS

The electronic structure of atoms refers to how electrons are arranged within an atom. The arrangement of electrons in an atom's orbitals is called its electron configuration. It significantly impacts an element's chemical behavior.

Electron Configuration

Terminologies Review:

Proton	• A positively charged atomic element.
Neutron	• A neutrally charged atomic element.
Nucleus	• The center of an atom, composed of the proton(s) and the neutron(s)
Electrons	• A negatively charged atomic element that orbits the nucleus.
Ion	• An atom that has either gained or lost an electron causes the atom to become either negatively or positively charged, respectively.
Valence Shell	• The outermost orbital shell of an atom.
Valence Electron	• The electron/s in the outermost orbital shell of an atom is called its valence electron/s.

Rutherford's Atomic Model

This model is also known as the nuclear model of an atom. It describes the atom in a model wherein the center is a nucleus composed of protons and neutrons, which contain most of its mass. The nucleus is surrounded by electrons, which occupy most of its volume. This model does not fully explain the behavior and arrangement of electrons in the space around the nucleus.

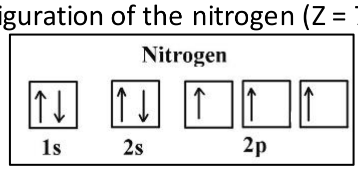
Bohr's Atomic Model

Niels Bohr, a Danish physicist, proposed a new model of the atom. He suggested that electrons do not emit energy while orbiting the nucleus but instead exist in stationary states with constant energy. This model is also called the planetary model of the atom. In this model, he proposed that the electrons encircle the nucleus in their respective orbits. The electrons are not allowed to occupy spaces in between the orbits. The farther the orbits from the nucleus, the higher the energy.

Hund's Rule

- Every orbital in a sublevel is singly occupied before any orbital is doubly occupied.
- All the electrons in singly occupied orbitals have the same spin (to maximize total spin).

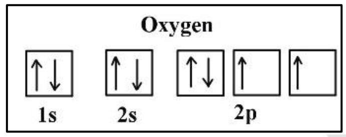
1. Consider the correct electron configuration of the nitrogen (Z = 7) atom: $1s^2\ 2s^2\ 2p^3$



The p orbitals are half-filled; there are three (3) electrons and three (3) p orbitals. It is because the three (3) electrons in the 2p subshell will fill all the empty orbitals first before pairing with electrons in them.

Keep in mind that elemental nitrogen is found in nature typically as dinitrogen, N_2, which requires molecular orbitals instead of atomic orbitals, as demonstrated above.

2. Consider the oxygen (Z = 8) atom, the element after nitrogen in the same period; its electron configuration is $1s^2\ 2s^2\ 2p^4$



Oxygen has one more electron than nitrogen; as the orbitals are all half-filled, the new electron must pair up. Keep in mind that elemental oxygen is found in nature typically as dioxygen, O_2, which has molecular orbitals instead of atomic orbitals, as demonstrated above.

Aufbau Principle

- As electrons are added to “build up” the elements, each electron is placed in the lowest energy orbital available (Aufbau is German for “building up”).

If we follow the pattern across a period from B (Z=5) to Ne (Z=10), the number of electrons increases, 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.

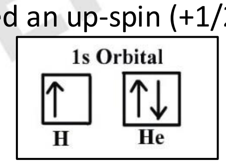
- B (Z=5) configuration: $1s^2\ 2s^2 2p^1$
- C (Z=6) configuration: $1s^2\ 2s^2 2p^2$
- N (Z=7) configuration: $1s^2\ 2s^2 2p^3$

- O (Z=8) configuration: $1s^2\ 2s^2 2p^4$
- F (Z=9) configuration: $1s^2 2s^2\ 2p^5$
- Ne (Z=10) configuration: $1s^2 2s^2 2\ p^6$

**Take note of the highlighted parts. The number of electron(s) depends on the element.*

Pauli Exclusion Principle

In an atom or molecule, no two (2) electrons can have the same four (4) electronic quantum numbers. As an orbital can contain a maximum of only two (2) electrons, the two (2) electrons must have opposing spins. It means if one is assigned an up-spin (+1/2), the other must be a down-spin (-1/2).



Rules for Determining Electron Configuration:

1. Each added electron enters the lowest energy orbital available (Aufbau Principle).
2. No more than two (2) electrons can be placed in any orbital. (Pauli-Exclusion Principle)
3. Before a second electron can be placed in any orbital, all the orbitals of that sub-level must contain at least one electron. Refer to Hund’s Rule.

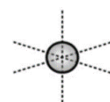
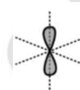
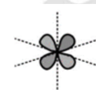
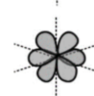
∴ The electron configuration code lists the number of the principal energy level followed by the letter of the sub-level type. A superscript is placed on the sub-level letter to indicate the number of electrons in that sub-level.

Examples:
Write and illustrate the unabbreviated electron configuration of the following elements.
1. Potassium - $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1$
2. Sodium - $1s^2\ 2s^2\ 2p^6\ 3s^1$
3. Copper - $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^1$
4. Nickel - $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^8$

Quantum Numbers

Quantum(pl. Qanta) is a quantity of energy involved in an interaction.
Quantum numbers describe the position and energy of the electron in an atom.

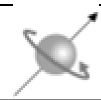
The Four Quantum Numbers
1. The principal quantum number **($\boldsymbol{n}$)** is the number of the energy level.
   - The larger the value of n, the farther it is from the nucleus and the higher its energy.
2. Azimuthal **($\boldsymbol{\ell}$)** indicates the subshell in which an electron can be found. It corresponds to the shape of the orbital

ℓ = 0	s-orbitals	spherical	
l = 1	p-orbital	Dumbbell shape	
l = 2	d-orbitals	clovers	
l = 3	f-orbitals	complex	

3. Magnetic quantum number **($\boldsymbol{m\ell}$)** describes the orientation in space of a particular orbital.
   - In bond formation, the magnetic quantum number determines how the elements will overlap depending on their orientation. The possible values for ml are:

ℓ = 0	s-orbitals	□	0
l = 1	p-orbital	□□□	-1, 0,1
l = 2	d-orbitals	□□□□□	-2, -1, 0, 1, 2
l = 3	f-orbitals	□□□□□□□	-3, -2, -1, 0, 1, 2, 3

4. Electron spin quantum number (m_s) indicates the orientation of the angular momentum of an electron in an atom.

Spin up	+1/2	
Spin down	-1/2	

Examples:

1. What are the possible subshells when n = 4? How many orbitals are contained by each of these subshells?
   Given: n = 4
   l = 0, 1, 2 or 3 = 4 subshells (s, p, d, f)
   ml = -4,-3, -2, -1, 0, 1, 2, 3, 4
2. Identify the four quantum numbers for the last valence electron of the Tungsten atom. Tungsten (W) = $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^{10}\ 5p^6\ 6s^2\ 4f^{14}\ 5d^4$
   *valence electron: $5d^4 \rightarrow$ n= 5, l = 2, ml = 1, ms = +1/2

Planck's Quantum Theory

- Proposed by Max Planck during the 19th century.
- Energy is always emitted in integral multiples of $h\nu$, postulated that the energy of a particular quantum of radiant energy could be described by the equation:

$$\mathbf{E = h\frac{c}{\lambda}}$$

Photoelectric Effect

- Contributed by Albert Einstein, five years after Planck presented his Quantum Theory.
- A phenomenon in which electrons are ejected from the surface of certain metals exposed to light of at least a certain minimum frequency.
- Particles of light are called photons, which possess energy.

$$\mathbf{E = h\nu}$$

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