Atomic structure

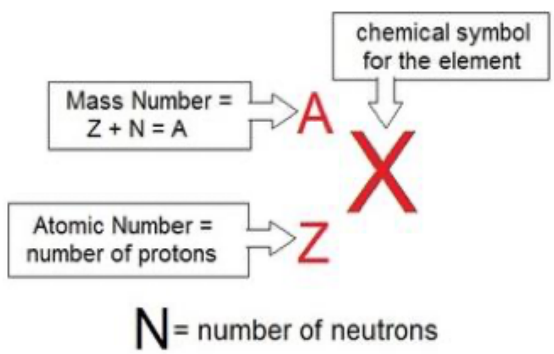
author: SAM RENXUYI

Table of contents

The nuclear atom

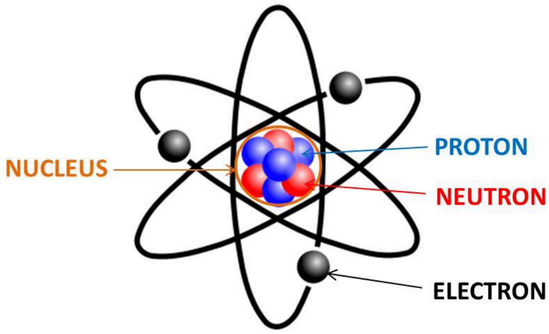
Atomic composition

- **Nucleus**: A positive charged, dense area composed of **protons** and **neutrons**
- **Electrons**: A particle (e^-, β^-)which contain 1 elementary charge and occupy the space **outside** the nucleus.
- **Mass number(A)**: Sum of the number of protons and neutrons in the nucleus
- **Atomic number (Z)**: The number of protons in the nucleus. Since atoms are electrically neutral, the number of protons is also equal to the number of electrons(**In atom not in ions**)
- **Isotope**: Atoms of the same element with the same number of protons, but with a different number of neutrons



Sub-atomic particle	relative mass	relative charge
Proton	1	+1
Neutron	1	0
Electron	$\frac{1}{1836}$	-1

Note that electrons are assumed to be **massless**



Properties of isotopes

- **Chemical properties** depend on the **outer shell of electrons**. Since isotopes still have the same number of electrons, these properties will **remain the same**
- **Physical properties** depend on their **nuclei**. Since the number of neutrons changes, properties such as **density, rate of diffusion, melting and boiling change. The mass will also change**

Uses of radioisotopes

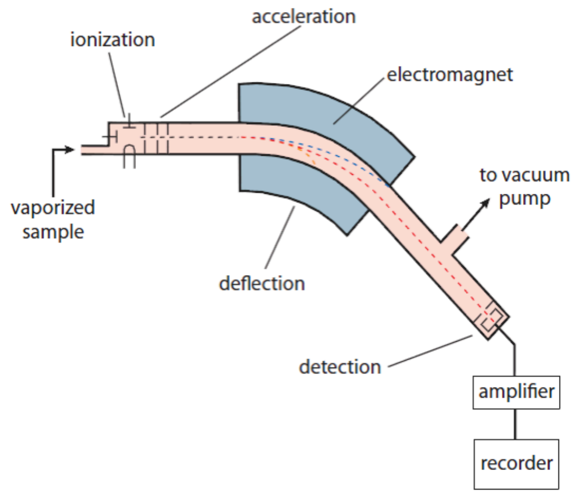
- **Carbon-14**: Carbon-14 is used to estimate the age of organisms. This process is called radiocarbon dating
- **Iodine-131/Iodine 125**: It can be used to treat thyroid cancer, and detect if the thyroid is functioning correctly, Iodine 125 is a gamma emitter and can treat prostate cancer and brain tumors. It is also taken up by the thyroid gland.

Mass Spectrometry(HL)

- A mass spectrometer is an instrument that can be used to measure the individual masses of atoms
- A mass spectrometer separates individual isotopes from a sample of atoms and determines the mass of each isotope
- The deflection or path of an ion in a mass spectrometer depends on:

    1. Absolute mass of the ion

2. Charge of the ion
3. Strength of magnetic field
4. Velocity



Calculating atomic mass(IMPORTANT)

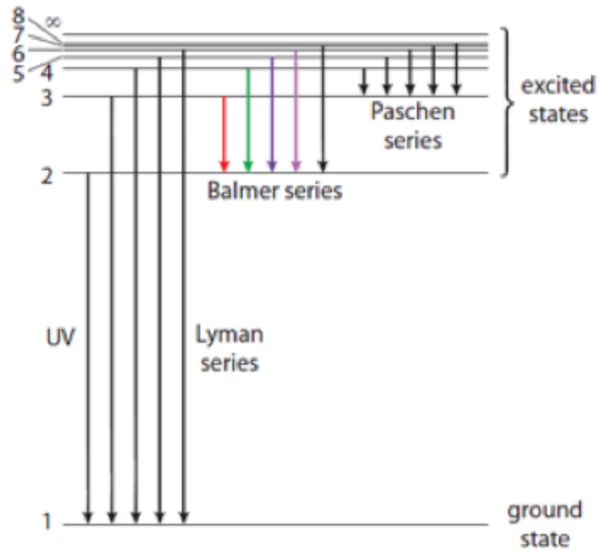
- As the relative atomic mass of an element is the weighted average of the relative masses of the isotopes of an element we can calculate relative atomic mass using the following formula:

$$A_r = \frac{(relative\ isotopic\ mass_1 \times \%abundance_1) + (relative\ isotopic\ mass_2 \times \%abundance_2) + \ldots}{100}$$

Electron configuration

Emission spectrums

Emission spectra are produced when photons are **emitted** from atoms as excited electrons return to a lower energy level.

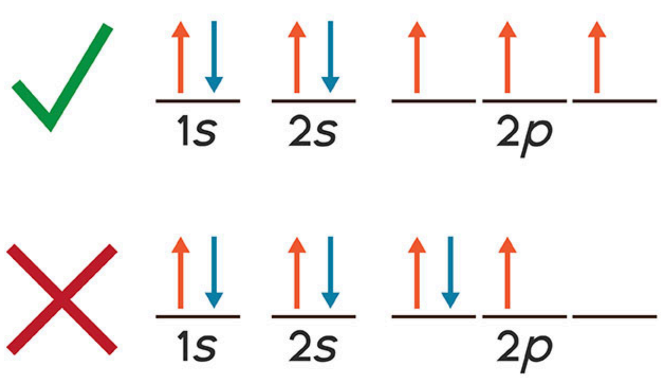


1. The emission which electron back to n=1 main level is UV lights
2. When n=2 it is visible light
3. When n=3 it is infrared.

Orbitals

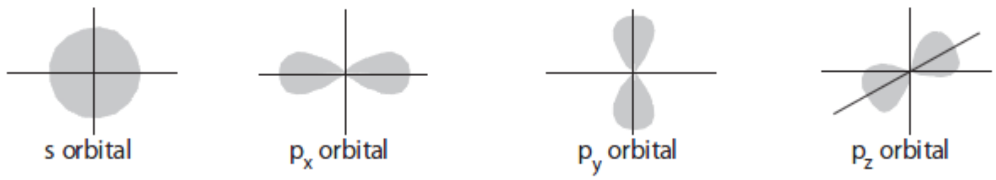
Three rules control how electrons fill atomic orbitals:

1. **Pauli's Exclusion Principle**: No more than two electrons can occupy any one orbital and if two electrons are in the same orbital they must spin in **opposite**
2. **Aufbau Principle**: Electrons are placed into orbitals of lowest energy first
3. **Hund's Third Rule**: Orbitals of the same sub-level are **filled singly first**, then doubly. If more than one orbital in a sub-level is available, electrons occupy different orbitals with parallel spins

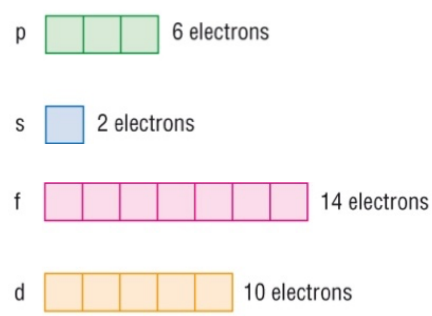


s p d f Sub-levels(Sub shells)

- **Orbitals can take up to 4 different shapes**
- 1. s-orbitals take a **spherical** shape
- 2. p-orbitals resemble a “**dumbbell**” shape

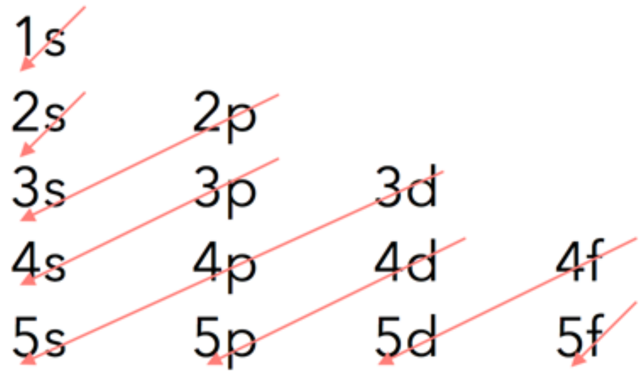


- The sub-levels s, p, d and f contain the following number of orbitals respectively where every orbital can hold up to two electrons maximum.
    - s: 1 orbital 2 electrons
    - p: 3 orbitals 6 electrons
    - d: 5 orbitals 10 electrons
    - f: 7 orbitals 14 electrons



- How to write an electron configuration?

1. Find out the number of electrons
2. Fill the orbitals one by one in a certain order, you can use the order below the text.
3. S-orbital can hold 2 electrons, each p-orbital can hold 6, each d-orbital can hold 10 and each f-orbital can hold 14



- IMPORTANT: **The 4s orbital is filled first before 3d, but is removed first before 3d**
- Another way to write the configration easily is write the symbol in square brackets ([X]) for the nearest, smaller noble gas (The square brackets represent the electron configuration for the noble gas), write the electron configuration following the noble gas configuration.
- Some Exception (**Must remember**)
    - Chromium has the electron configuration: [Ar] $3d^5 4s^1$
    - Copper has the electron configuration: [Ar] $3d^{10} 4s^1$

Electrons in atoms

Definitions of First Ionization energy (IMPORTANT)

- The **minimum** amount of energy required to **remove one mole of electrons** from **one mole of gaseous atoms**. The formula for first ionization energy is: $X_{(g)} \rightarrow X^+{}_{(g)} + e^-$

The meaning of convergence line in a spectrum

- In an emission spectrum, the limit of convergence at higher frequency corresponds to the first ionization energy

The factors of First ionization energy

Size of the nuclear charge

- As the atomic number (**number of protons**) **increases, the nuclear charge increases**
- The larger the positive charge, the greater the attractive electrostatic force between the nucleus and all the electrons
- So, a larger amount of energy is needed to overcome these attractive forces and remove an electron
- As the proton number increases, ionization energy increases: First ionization energy increases across each period

The distance between the electrons and nucleus

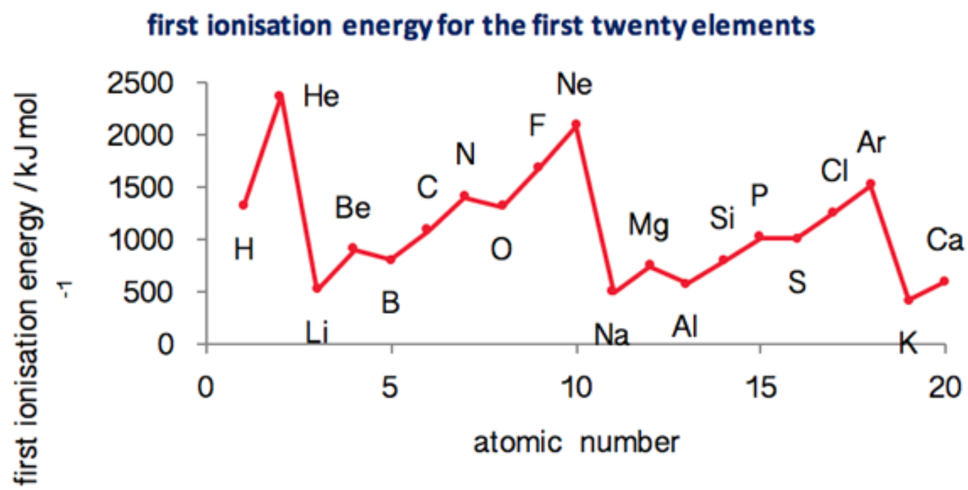
- The force of electrostatic attraction between positive and negative charges **decreases** rapidly **as the distance between them increases**
- Hence electrons in shells (main energy levels) further away from the nucleus, **are more weakly attracted to the nucleus than those closer to the nucleus**
- The **further the outer electron shell** is from the nucleus, **the lower the ionization energy**
- Thus, ionization energies tend to decrease down a group of the periodic table

Shielding effect

- Since all electrons are negatively charged, **they repel each other**
- Electrons in full inner shells repel electrons in outer shells
- The full inner shells of electrons prevent the full nuclear charge being experienced by the outer electrons. This is known as **shielding**
- The **greater the shielding of outer electrons by the inner electron shells**, the **lower the electrostatic attractive forces** between the nucleus and the outer electrons

- The ionization energy is **lower** as the **number of full electron shells** between the outer electrons and the nucleus **increases**

Graph of First ionization energy

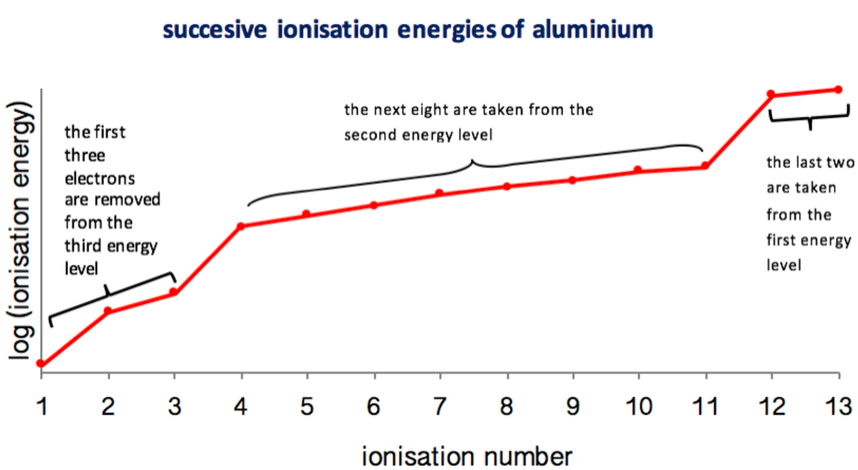


- The general trend is that first ionization energies **increase from left to right across a period**
- The increase in nuclear charge across a period causes an increase in the attraction between the outer electrons and the nucleus makes the electrons **more difficult to remove**
- However, 1st I.E.(First ionization energy) sometimes drops between elements in periods, (Be to B). This is because Beryllium has the electronic structure 1s2 2s2 and the boron atom has the electronic structure $1s^2\ 2s^2\ 2p^1$.
- 1st I.E. will decrease as the electron is being removed from the s-orbital in Be whereas for B it is being removed from the p-orbital which has a slightly higher energy and this counteracts the increase in effective nuclear charge
-
    - **The greater the nuclear charge on the atom the harder it is to remove an electron**
    - **Sub-levels are more stable when they are empty, half-full or full**
    - **Electrons prefer to be unpaired if possible as pairing of**

electrons creates repulsion

Successive ionization energies

- The second and third ionization energies are described as:
  - $X_{(g)}{}^{+} \rightarrow X^{2+}{}_{(g)} + e^{-}$
  - $X_{(g)}{}^{2+} \rightarrow X^{3+}{}_{(g)} + e^{-}$
- Successive ionization energies increase for all atoms because as more electrons are removed the remaining electrons experience an increasing effective nuclear charge and are held closer to the nucleus and hence more tightly
- **The large increases (jumps) in**
- **Successive ionization energies increase for all atoms** because as more electrons are removed the remaining electrons experience an **increasing effective nuclear charge** and are **held closer to the nucleus** and hence more tightly
- **The large increases (jumps) in ionization energy correspond to a change to a new inner shell**, closer to the nucleus, with the electrons held more strongly



Caculate the I.E. by the convergence line

- We can use the ionization energy data to determine the wavelength of frequency of convergence.
- And we can caculate the energy or wavelength by the following formula:

  $c = v\lambda$ and $E = hv$
- h is Planck's constant $6.63 \times 10^{-34}\ Js$
- c is the speed of light $3.00 \times 10^{8}\ ms^{-1}$