Inorganic Chemistry

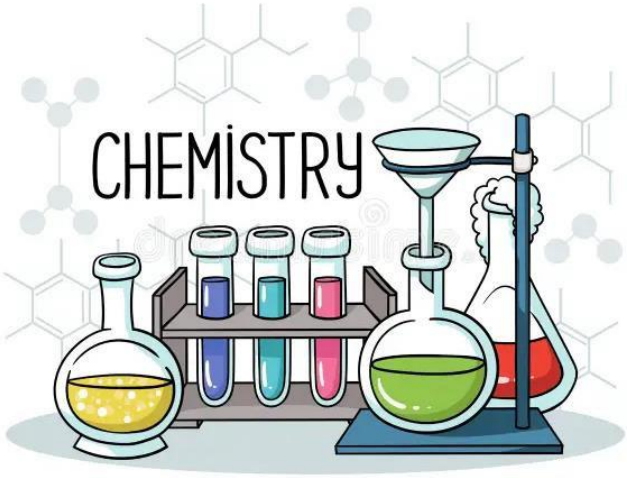
Textbook

For

First year - Chemistry Students

By

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Inorganic Chemistry

Dr.Sarab Alazawi **2026-2027** **first year**

Basic information

Chemistry Is a whole branch of science about ***matter***, which is anything that has mass and occupies space. ***Chemistry*** is the study of the composition and properties of matter and the changes it undergoes.

Branches of Chemistry

1- **Organic Chemistry** involves the study of the structure, properties, and preparation of chemical compounds that consist primarily of carbon and hydrogen.

2-**Inorganic Chemistry** is the study of the properties and behaviour of inorganic compounds. It covers all chemical compounds except organic compounds. Inorganic chemistry study things such as crystal structures, metals, catalysts, and most elements in the Periodic Table**.**

3- **Analytical Chemistry:** involves the qualitative and quantitative determination of the chemical components of substances.

4- **Physical Chemistry**: The study of the effect of chemical structure on the physical properties of a substance.

5- **Biochemistry:** The study of chemical reactions that take place in living things. It tries to explain them in chemical terms**.**

Atomic structure

The ***atom*** is the smallest part of matter that represents a particular element.

The atoms of a particular element can have an identical number of protons and electrons but

varying numbers of neutrons. If they have different numbers of neutrons, then the atoms are called ***isotopes (****Atoms of the same element that have same atomic number* but *different numbers of* ***neutrons)***. The figure below shows the three hydrogen isotopes, *Hydrogen* or (**Protium**) has (1p + 0N), ***Deuterium*** has (1p + 1N) and ***Tritium*** has (1p +2N).

There are three major atomic particles: ***Protons***, ***Neutrons*** and ***Electrons***. Table below summarizes the characteristics of these three subatomic particles. The masses of subatomic particles are listed in two ways: grams and atomic mass units (AMUs). Expressing mass in amu is much easier than using the gram equivalent.

Name	Symbol	Charge	Mass (*g*)	Mass (*amu*)	Location
Proton	P^+	**+1**	1.673×10^{-24}	**1**	**inside nucleus**
Neutron	N^0	**0**	1.675×10^{-24}	**1**	**inside nucleus**
Electron	e^-	**-1**	9.109×10^{-28}	**0.0005**	**Outside nucleus**

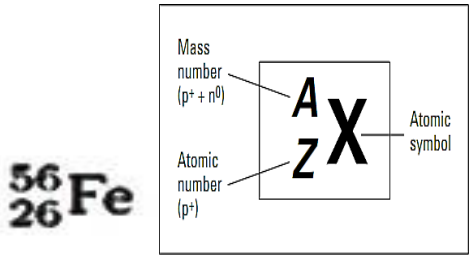
Inorganic Chemistry

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One **atomic mass unit** is defined as a mass exactly equal to one twelfth the mass of one carbon -12 atom. And 1 amu = 1.66056×10^{-24} g Mass of an atom of hydrogen = 1.6736×10^{-24} g Thus, in terms of amu, the mass of hydrogen atom = $1.6736 \times 10^{-24} / 1.66056 \times 10^{-24}$ = 1.0078 amu = 1.0080 amu. Similarly, the mass of the oxygen-16 (16O) atom would be 15.995 amu. Today, **'amu'** has been replaced by **'u'** which is known as **unified mass**.

Atomic number (Z): The number of protons in the nucleus of an atom. In electrically neutral atoms, this number is also equal to the number of electrons orbiting about the atom's nucleus. For example H =1, Br =35, Cl= 17

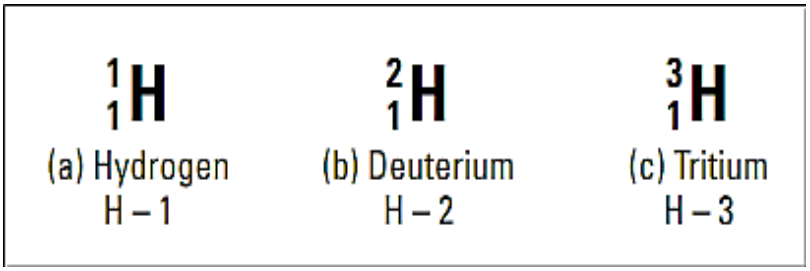
Mass numbers (A): is the total number of **protons** and **neutrons** in an atomic nucleus.



The iron nucleus which has 26 protons and 30 neutrons, is denoted as Where the total atomic number is (Z = 26) and the mass number (A = 56). The number of **neutrons** is simply the difference (**N = A – Z**) **56-26 =30**

Isotopes:-

atoms with identical atomic number but different atomic mass number are known as Isotopes. It is evident that difference between the isotopes is due to the presence of different number of neutrons present in the nucleus. For example, considering of hydrogen atom again, 99.985% of hydrogen atoms contain only one proton. This isotope is called protium($^{1}_{1}H$). Rest of the percentage of hydrogen atom contains two other isotopes, the one containing 1 proton and 1 neutron is called deuterium ($^{2}_{1}D$, 0.015%) and the other one possessing 1 proton and 2 neutrons is called tritium ($^{3}1T$).



Other examples

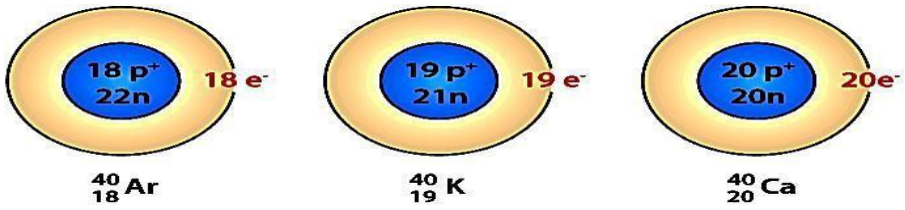
Element	Isotopes
Carbon (C)	$^{12}_{6}C$, $^{13}_{6}C$, $^{14}_{6}C$
Nitrogen (N)	$^{14}_{7}N$, $^{15}_{7}N$,
Oxygen (O)	$^{16}_{8}O$, $^{17}_{8}O$, $^{18}_{8}O$
Chlorine(Cl)	$^{35}_{17}Cl$, $^{37}_{17}Cl$
Uranium (U)	$^{235}_{92}U$, $^{238}_{92}U$, $^{239}_{92}U$
Sulphur (S)	$^{32}_{16}S$, $^{33}_{16}S$, $^{34}_{16}S$, $^{36}_{16}S$

Lastly an important point to mention regarding isotopes is that chemical properties of atoms are controlled by the number of electrons, which are determined by the number of protons in the nucleus. Number of neutrons present in the nucleus have very little effect on the chemical properties of an element. Therefore, all the isotopes of a given element show same chemical behaviour.

Each of these isotopes have different abundance in nature. The table below outlines the average isotopic abundances of elements that are most commonly measured for stable isotope measurements.

Hydrogen	Carbon	Nitrogen	Oxygen
^{1}H – 99.984%	**^{12}C – 98.89%**	**^{14}N – 99.64%**	**^{16}O – 99.763%**
^{2}D – 0.0156%	**^{13}C – 1.11%**	**^{15}N – 0.36%**	**^{17}O – 0.0375%**
----	**----**	**----**	**^{18}O – 0.1995%**

Isobars: are atoms of different elements that have the same number of mass number, but they have different atomic number



Isotones: Are different atoms that have the same number of neutrons and Different number of protons.

$$\text{Isoton} = {}^{14}_{7}N,\ {}^{13}_{6}C,\ {}^{15}_{8}O$$

Stable vs. Unstable Isotopes

There are two types of isotopes, one which is found in nature, stable and not radioactive, the second type is the one which is naturally radioactive and not stable. Any element having excess of neutrons in the nucleus as compared to the stable form of atom tends to be unstable in nature. These elements tend to be radioactive and undergo radioactive decay by emitting energy.

Unstable nuclei decay by giving off ***Alpha*** particles (helium nuclei), ***Beta*** particles (electrons or antielectrons) or ***Gamma*** particles (photons of high energy electromagnetic radiation).

Relative atomic mass (RAM)

The relative atomic mass of an atom is the weighted average of the masses of isotopes.

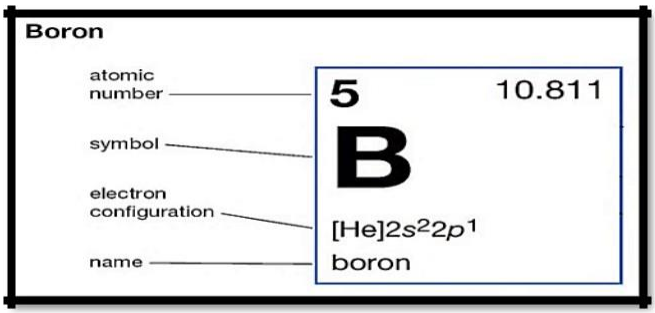
$$\text{RAM} = \frac{\text{(Mass of 1st isotope)*(Its abundance \%)] + [(Mass of 2nd isotope)*(Its abundance \%)] + (etc....)]}}{100}$$

Example: The natural abundance for Boron isotopes is 19.9% ^{10}B (10.013 amu*) and 80.1% ^{11}B (11.009 amu*). Calculate the relative atomic mass of boron.

$$RAM = \frac{\text{(Mass of 1st isotope)*(Its abundance \%)] + [(Mass of 2nd isotope)*(Its abundance \%)] + (etc....)]}}{100}$$

$$\textbf{(RAM)} = \frac{[(10.013) * (19.9\%)] + [(11.009) * (80.1\%)]}{100} = \textbf{10.811}$$

(Note: - that this is the value of atomic mass given on the periodic table).



Example: Calculate RAM for naturally occurring Mg if the isotope distribution is 78.99% ^{24}Mg, 10.00% ^{25}Mg and 11.01% ^{26}Mg; accurate masses are 23.99, 24.99 and 25.98.

(RAM) = [(23.99)*(78.99%)] + [(24.99)*(10.0%)] + [(25.98)*(11.01%)] 100

= **24.30**

H.W. Calculate the value of RAM for naturally occurring chlorine if the distribution of isotopes is 75.77% $^{35}_{17}Cl$ and 24.23% $^{37}_{17}Cl$. accurate masses for ^{35}Cl and ^{37}Cl are 34.97 and 36.97. **[Ans. 35:45]**

How to calculate the abundance of isotopes

We can let **X** represent the fractional abundance for **isotope 1** and **(1-X)** represent the fractional abundance for **isotope 2**.

Q/ Rabidium has two isotopes. ^{85}Rb has mass 84.9117 amu and ^{87}Rb has mass 86.9085amu. if the relative atomic mass is 85.4678 amu. What is the abundance of each isotopes?

isotope	mass	% suggestion	Abundance

^{85}Rb	84.9117 amu	x	?
^{87}Rb	86.9085 amu	1-x	?

85.4678= (84.9117) (x) + (86.9085) (1-x)
85.4678= 84.9117x+ 86.9085- 86.9085x
85.4678-86.9085= 84.9117x- 86.9085x
-1.4407= -1.9968x
X= 0.7215
%= 72.15 of ^{85}Rb
1-x = 1-0.7215= 0.2785= 27.85% of ^{87}Rb

Electromagnetic Radiation

James Maxwell (1870) was the first to give a comprehensive explanation about the interaction between the charged bodies and the behaviour of electrical and magnetic fields on macroscopic level. He suggested that when electrically charged particle moves under accelaration, alternating electrical and magnetic fields are produced and transmitted. These fields are transmitted in the forms of waves called electromagnetic waves or electromagnetic radiation. An electromagnetic radiation may be defined as the radiant energy which is transmitted through space at enormous velocities. It exists in various forms; the visible light and radiant heat being the easily recognized forms which we experience in day today life too. Unlike sound, EM radiation does not require a medium for transmission and passes readily through a vacuum; in a vacuum, the velocity of radiation is 3×10^8 m s^{-1}. The properties of electromagnetic radiation could be explained in terms of both the classical wave model (wave mechanics) and the particle model (quantum mechanics).

Wave Mechanical Model of Electromagnetic Radiation

In the wave mechanical model, the electromagnetic radiation is considered to be sinusoidal in nature, i.e., varying like a sine function. According to the Maxwell's theory, an electromagnetic wave can be visualized as oscillatory electric and magnetic fields travelling in the planes perpendicular to each other and also to the direction of propagation (Fig. 1.).

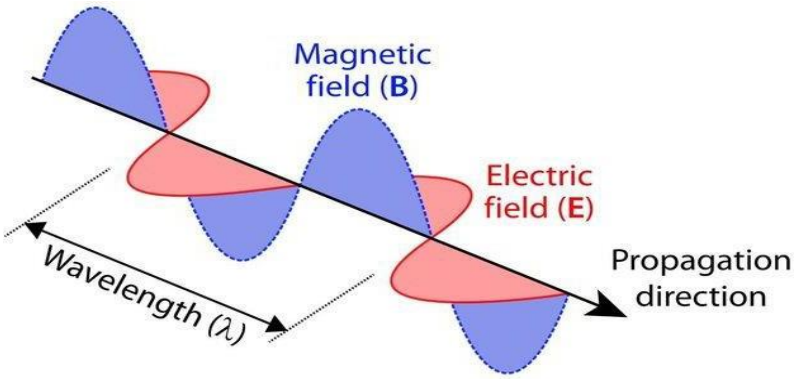


Figure1: An EM radiation showing oscillatory electric and magnetic fields

Dual Nature of Light

Theories of nature of light

There are four important theories to explain the nature of light

Newton's Corpuscular Theory

This theory was put forward by Newton in 1678 AD. According to this theory, light consists of small particles called 'Corpuscles'. These small particles are produced by luminous sources. They travel in all direction with high velocity. This theory tried to explain the phenomena of refraction of light. This theory fails to explain phenomena like interference, diffraction etc.

Wave theory

In 1690, physicist Christian **Huygens** proposed wave theory of light. According to this theory, light is from of energy and travels as a wave. Each point of light acts as a source and sends wave in all direction. In 1801, **Thomas Young** demonstrated the interference of two light beams which is strong evidence for the wave theory of light. This theory successfully explained reflection, refraction interference and diffraction. Huygens considered light as a wave travelling in a hypothetical medium called Aether. Later, **Young and Fresnel** assumed light as a wave.

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Electromagnetic theory

In 1860 AD, from basic four Maxwell equations, Maxwell found a mathematical expression for the speed of electromagnetic waves. Where is the permeability and is the permittivity of the space. In a vacuum, this value was calculated to be m/s. This is exactly the speed of light observed from the experiment. Maxwell suggested that this isn't coincidence rather light is an electromagnetic wave. An electromagnetic wave consists of changing electric and magnetic fields which are perpendicular to each other. So, the light wave is transverse in nature.

Quantum theory of radiation

Wave theory of light couldn't explain certain phenomena such as photoelectric effect, atomic excitation, Compton Effect etc. In 1905 AD, Albert Einstein proposed a new theory of light called quantum theory based on the assumptions of Max Planck. According to this theory, light consists of a tiny packet of energy called quanta or photons. The energy of each 'Quanta' given by;

$E = h V$

E = Energy of each quanta

h = Planck's constant

υ = frequency of radiation

The absorption and the release of energy is always in the integral multiple of this energy.

Characteristic of electromagnetic radiation

1. These consist of electric and magnetic fields that oscillate in the directions perpendicular to each other.
2. All electromagnetic waves travel with same velocity. $3x10^8$ m/sec.
3. These electromagnetic radiations do not require any medium for propagation. E.g. light reaches us from the Sun through an empty space.

Properties of Waves and Electromagnetic radiation

Any wave was characterized by its wavelength and frequency

Wave length (λ)

The wavelength denoted by λ (lambda) is defined as the distance between any two adjacent peaks (crests) or troughs on successive waves. Unit – A^0 (Angstron) $1A^0 = 10^{-8}$ cm = 10^{-10} m SI unit: μ (micrometer), mμ (milli micron), nm (nanometer), pm (picometer). $1A^0 = 10^{-10}$m; $1\mu = 10^{-6}$ m; $1m\mu = 10^{-9}$ m $1nm = 10^{-9}$ m; $1pm=10^{-12}$m

Frequency (ν)

The frequency, ν (nu) is the number of waves or cycles per second pass through a given point. In following figure shows the frequency corresponds to the number of times per second that moves through a complete cycle of upward and downward motion. The frequency is expressed in the unit of cycles per second (s^{-1}) or Hertz (Hz). 1 Hz = 1 cycles per second $\nu = C/\lambda$

Unit	Frequency, (cycles/sec)
Hertz, Hz	**1**
Kilohertz, KHz	**10^3**
Megahertz, MHz	**10^6**
Gigahertz, GHz	**10^9**

Amplitude It is the vertical distance from the midline of a wave to the peak or trough. Height of crest or depth of trough i.e. intensity or brightness.

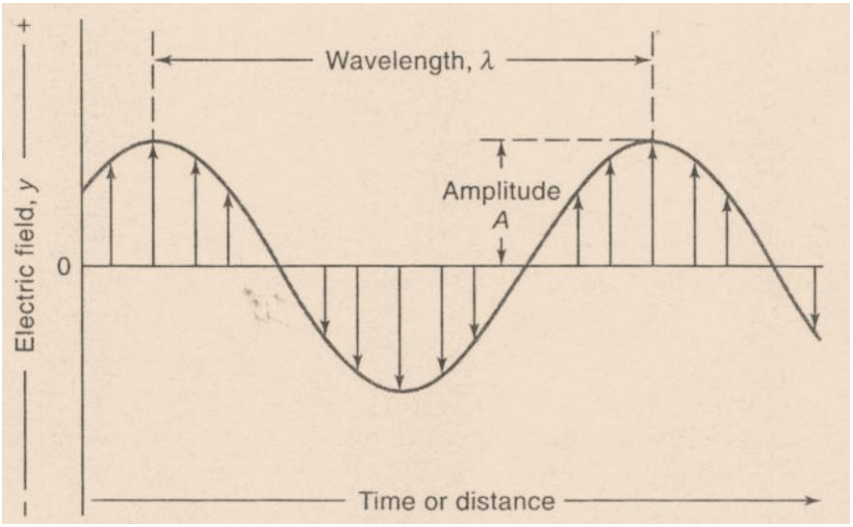
Velocity (C)

Distance travelled by a light in one second. The unit of velocity is ms^{-1} or cms^{-1}

Wave number ($\bar{\upsilon}$)

The number of waves per unit length. Unit: cm^{-1} or m^{-1}, $\bar{\upsilon} = 1/\lambda$

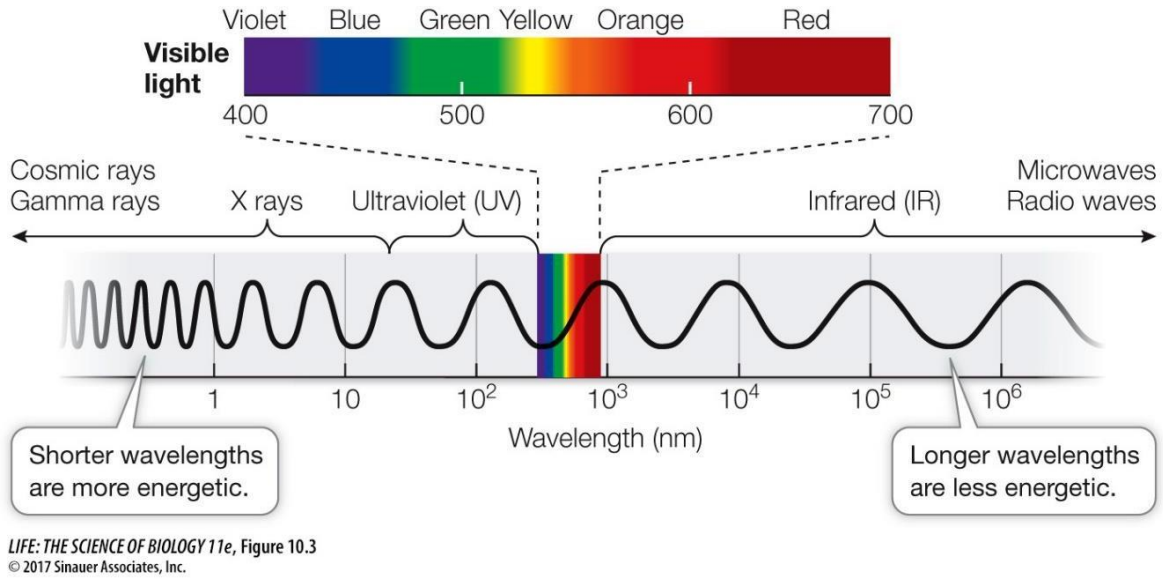
Relationship: $C = \lambda \times \nu$; $\nu = C/\lambda \rightarrow \nu = C\,\bar{\upsilon}$



Exercise.1 Calculate the speed of a wave whose wavelength and frequency are 17.4cm and 87.4 Hz, respectively. This is directly solved by the application of $c = \lambda\nu$ $c = 17.4$ cm x 87.4 Hz; $c = 17.4\text{cm} \times 87.4/\text{s} = 1.52 \times 10^3$ cm/sec

The Electromagnetic Spectrum

Depending on the wavelengths, electromagnetic radiation is of many types and constitutes called an electromagnetic spectrum. The EM spectrum is divided into different regions on the basis of the methods required to generate and detect them. The radiations of different regions differ in terms of their characteristics like energy, wavelength, etc. The electromagnetic spectrum is divided into γ-rays, x-rays, ultraviolet, visible, infrared, microwave and radio waves, etc. in terms of increasing wavelengths.



LIFE: THE SCIENCE OF BIOLOGY 11e, Figure 10.3
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The visible region of the spectrum which the human eye can sense is very tiny, as compared to the other spectral regions. Since the range of electromagnetic spectrum is quite large. The sources of radiation mostly give EM radiation spread over a range. In other words, the EM radiation emitted by the source contains a number of radiations having slightly different wavelengths. For example, a hot deuterium lamp emits radiations in the wavelength range of approximately 190-380 nm. Such a radiation is called polychromatic radiation signifying that it consists of many radiations of different wavelengths. We can generate or separate out radiation of a single wavelength from polychromatic radiation using a suitable device called a monochromator.

Gamma-rays: Gamma rays have the highest frequency and photon energy in the electromagnetic spectrum. They have extremely short wavelengths and are associated with nuclear processes and high-energy particle interactions.

X-rays

X-rays have frequencies and photon energies slightly lower than gamma rays. They are widely used in medical imaging, security screening, and industrial applications due to their ability to penetrate materials and reveal internal structures.

Ultraviolet (UV) Rays

Ultraviolet rays have higher frequencies and photon energies than visible light. They are emitted by the Sun and play a crucial role in biological processes, such as vitamin D synthesis and triggering chemical reactions in the atmosphere.

Visible Light

Visible light is the portion of the electromagnetic spectrum visible to the human eye. Visible light is essential for vision. It has a range of frequencies and photon energies that allow us to perceive different colours. we can see these waves as the colours of the rainbow where each colour includes a different wavelength. Red has the longest wavelength and violet has the shortest one. When all the waves are seen together, they form white light. When white light comes through the prism, it gets broken into the colours of the visible light spectrum.

Color Region	Wavelength (nm)
Violet	380-435
Blue	435-500
Cyan	500-520
Green	520-565
Yellow	565-590
Orange	590-625
Red	625-740

Infrared (IR) Rays

Infrared rays have lower frequencies and photon energies than visible light. They are associated with thermal radiation and are commonly used in night vision, remote sensing, and infrared spectroscopy applications.

Microwaves

Microwaves have slightly higher frequencies and photon energies than radio waves. They are commonly used in microwave ovens, satellite communication, and wireless technologies. Understanding the electromagnetic spectrum allows us to explore the diverse range of electromagnetic radiation and its applications.

Radio Waves

Radio waves have the lowest frequencies and photon energies in the electromagnetic spectrum. They are used for communication, broadcasting, and radar systems. Different portions of the radio wave spectrum are allocated for various applications, including AM and FM radio, television, and mobile communication.

Planck's Quantization Energy

Max Planck found a theoretical formula that exactly describes the intensity of light of various frequencies emitted by a hot solid at different temperatures. According to Planck, the atoms of the solid oscillate, or vibrate with a definite frequency,ν depending on the solid and he found it necessary strong idea.

1. Radiant energy is not emitted or absorbed continuously but discontinuously in the form of small pockets of energy called quanta. Each such quanta is associated with a definite amount of energy. In the case of light, the quanta of energy are often called photon.

2. The amount of energy associated with a quantum of radiation is proportional to the frequency of light. E∝ ν or E = h ν and where, h is a Planck's constant with the value 6.63 x 10^{-34} J.s. This relation found to be valid for all type of electromagnetic radiation.

3. The total amount of energy emitted or absorbed by a body (matter) will be some whole number multiple of quantum. E= nhν ---------- (1) n=1,2,3,…..... This means that a body can emit or absorb energy equal to hν, 2hν, 3hν, ... Or any other integral multiple of hν. But cannot emit or absorb fractional value of hν. We know that,

$$c = v \times \lambda$$

$$v = \frac{c}{\lambda}$$

Equations (1) and (2) give the relation between energy of radiation and its frequency or wavelength

E= h C/λ ----------(2).

A radiation which has higher the frequency or lowers the wavelength has more energy. For example, violet light is larger frequency has more energy than red light which is having lower frequency.

Problem1: A dental hygienist uses x-rays (λ= 1.00Å) to take a series of dental radiographs while the patient listens to a radio station (λ = 325 cm) and looks out the window at the blue sky (λ= 473 nm). What is the frequency (in s^{-1}) of the electromagnetic radiation from each source? (Assume that the radiation travels at the speed of light, 3 x10^{8} m/s)?

Note: Converting from angstroms A to meters m

$\lambda = 1.00$ Å x 10^{-10} m = 1.00 x 10^{-10} m

For the x-rays

$$v = \frac{c}{\lambda} = \frac{3 \times 10^8}{1 \times 10^{-10}} = 3 \times 10^{18}$$

For the radio signal:

$$v = \frac{c}{\lambda} = \frac{3 \times 10^8}{325 \times 10^{-2}} = 0.00923 \times 10^{10}$$

For blue sky:

$$v = \frac{c}{\lambda}$$
$$= \frac{3 \times 10^8}{473 \times 10^{-9}}$$
$$= 0.0063 \times 10^{17}$$

Spectrum

When white light from Sun is passed through a prism, it split into a series of color band known as rainbow colors (VIBGYOR). This means that Sunlight is composed of collection of electromagnetic waves having different wave length. The splitting of light into seven colors is known as dispersion and the series of color bands is called a spectrum. In this spectrum, there is continuity of colors such a spectrum is known as continuous spectrum.

Atomic Spectra

Unlike the spectrum obtained by analyzing the sunlight, the spectra of atoms of elements can be made to emit energy by subjecting them to electric discharge or by heating are not continuous (discontinuous). The spectrum of atoms consists of sharp well-defined lines or bands corresponding to definite frequencies. There are two types of atomic spectra.

1- **Emission Spectra**

Emission spectra are obtained when the radiations emitted from substances are analyzed with the help of spectroscope. When the gases or vapor of chemical substances are analyzed with heated by electric spark, light is emitted. The color of light depends upon the substance under

investigation. Example, sodium gives a yellow light and potassium produces violet color. This type of spectrum consists of sharp welled fined line each corresponding to a definite frequency (or wavelength). Such spectrum is called line spectrum of discontinuous spectrum. The line spectrum also known as atomic spectrum because, it is obtained from atoms by the application of heat or other energy (electric). Example, Sodium always gives lines at 589nm and 589.6nm (yellow). From this reason line spectra are also called as finger prints of atoms.

2- Absorption Spectra

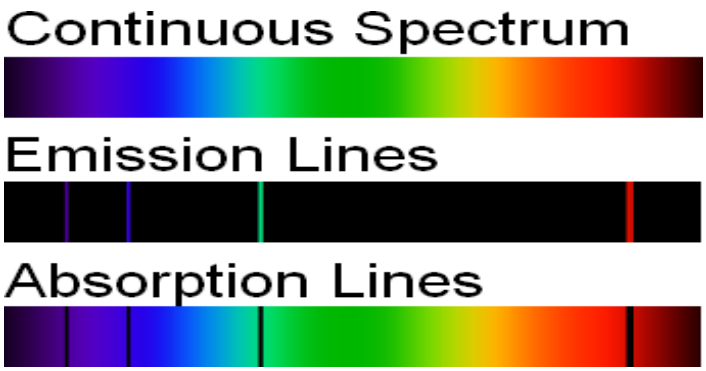
When a continuous electromagnetic radiation (white light) is allowed to pass through a gas or a solution of some salt and the transmitted light is analyzed. We obtain a spectrum in which dark lines are observed. These dark lines indicate that the radiations of corresponding wavelength have been absorbed by the substances from the white light. The dark lines of wavelengths are also character of a substance. Example, absorption of Na consists of lines at 589nm and 589.6nm same as that of emission spectrum.

Emission spectrum	Absorption spectrum
1-It is created when the atom of an element released energy	1-it is created when the atoms of an element absorb energy
2-Constitutes of coloured lines which can be seen in the spectrum	2-it constituents the dark lines in spectra
3-It can be used to drive the composition of specific metrial	3-it is helpful in figuring out capability of materials to retain heat
4-The type of particales of photons which are emitted can be used to figure but the kind of element a certain material is made up of as each elemnt has a unique level of energy Emission	4-The frequency of the light absorbed by the substance can tell us about the number of substances in sample

The emission or absorption spectrum is included of three types.

1. Continuous spectrum
2. Line spectrum- atomic spectra
3. Band spectrum- molecules spectra

Note: Continuous spectrum contains no gaps whereas line spectrum contains many gaps.



Emission Spectrum of hydrogen atom

The spectrum of hydrogen atom has played a very important role in the development of atomic structure. The spectrum of hydrogen atom can be obtained by passing an electric discharge current through the hydrogen gas taken in the discharge tube under low pressure. The emitted light (radiation) is analyzed by spectroscope. The spectrum consists of large number of lines appearing in different wavelengths (visible, UV, IR regions). In 1885, J.J.Balmer developed a relationship among the different wavelengths, λ in the visible region in hydrogen spectrum, could be reproduced by simple formula: i.e.

$$\bar{\upsilon} = \frac{1}{wavelength} = \frac{1}{\lambda}$$

$$\bar{\upsilon} = \frac{1}{\lambda} = R_H\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \qquad n2=3,4,5 \ \ldots\ldots\ n2>n1$$

where R_H, was a constant and n1=2 and n2 an integer greater than 2.

The value of R, fitting this relation is $1.09677 \times 10^7\ m^{-1}$ and is known as the Rydberg constant.

These series of lines which appear in visible region are named as Balmer series. Afterwards, a series of spectral lines of H_2 atom in different regions were discovered. These series of lines named after the name of its discoverers. These are Lyman, Balmer, Paschen, Brackett and Pfund series. Lyman – UV region; Balmer – Visible Paschen, Brackett and Pfund – IR region.

As the other series of hydrogen spectral lines were discovered, a more general expression was found by Rydberg, and is known as Rydberg equation derived as,

$E = - RH / n^2$---------- (1) n = 1,2,3,.., ∝ (for hydrogen)

atom) Where, RH is Rydberg constant has the value $2.18x10^{-18}$J, n is principal quantum number negative sign indicates arbitrary convention. The energy levels of the electron in the hydrogen atom do undergo a transition of electron between energy levels; electron loses energy, which is emitted as photon. The difference between the energies of the initial and final state is:

$\Delta E = E_f – E_i$, $E_f = - R_H (1/n_f^2)$ and $Ei = - R_H (1/ni^2)$ Therefore,

Because this transition results in the emission of a photon of frequency, ν and energy hν, we can write:

$$\Delta E = h\upsilon = -2.18 \times 10^{-18}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) \quad \text{J/atom}$$

$$\Delta E = E_{n_2} - E_{n_1}$$

$$\Delta E = -2.18 \times 10^{-18}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)\frac{J}{atom}$$

$$\Delta E = 13.6\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)\frac{eV}{atom}$$

When a photon is emitted, ni > nf. Consequently, the term is negative and ΔE is positive. When energy is absorbed, ni < nf and the term is positive, so ΔE is positive. The brightness of a spectral line depends on how many photons of the same wavelength are emitted. In equation (3) by substituting (R_H=2.18x10^{-18}J, h=6.623x10^{-34} J.sec.) and C=3x10^8 m/sec, we found that R_H/hC is 1.097x10^7 m, which is the constant given in the Balmer equation. The emission spectrum of hydrogen includes a wide range of wavelengths from the IR to UV, and lists the series of transitions in the hydrogen spectrum; they are named as

Series	n_f	n_i	Spectrum region
Lyman	1	2, 3, 4, . . .	Ultraviolet
Balmer	2	3, 4, 5, . . .	Visible and ultraviolet
Paschen	3	4, 5, 6, . . .	Infrared
Brackett	4	5, 6, 7, . . .	Infrared

The above equation (3), and lines only applicable for hydrogen atom. But other atoms lines are complicated and equation is also not obeyed. The energy levels of hydrogen atom with series of emission spectral transition are labeled with their principal quantum numbers. The spectrum of hydrogen atom holds the key to the inner structure of atom. Bohr proposed the theory of atom based on Planck's quantum theory and spectra of hydrogen atom. It can calculate the energy of electron in any orbit by equation.

$$E_n = R_H\left(\frac{Z^2}{n^2}\right)$$

R_H constant has another value like

R_H= -2.18*10^{-18}J/atom

R_H= -13.6 e.v/atom

The energy change of the electron between two orbits according to the equation below

$$\Delta E = E_{n_2} - E_{n_1}$$

Example: determine the wave length, frequency and energy of the fifth line of Lyman series and the third line of Balmmer series.

1- $$\bar{\upsilon} = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

n_1= 1, n_2 = 1+5= 6 Wave number $\bar{\upsilon}$= 109678(1/1^2 - 1/6^2) = 3046.47 cm^{-1}= $\frac{1}{\lambda}$= λ= 32*10^{-5} cm

2- $$v = \frac{c}{\lambda}$$

3- $$E = hv$$

Balmmer series n1= 2, n_2= 2+3= 5

$$\bar{\upsilon} = 109678 cm^{-1}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

$$\bar{\upsilon} = 109678 cm^{-1}\left(\frac{1}{2^2} - \frac{1}{5^2}\right) = \ 23032.38 cm -$$

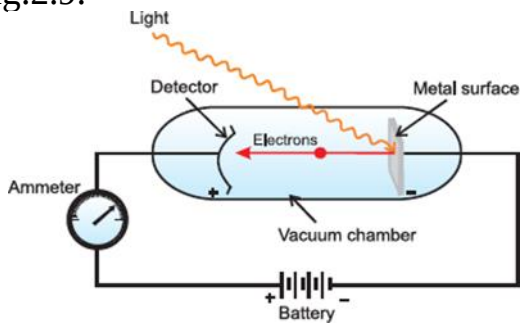
Note

1 erg =1.0 × 10^{-7} joules
E(J) = E(eV) × 1.602 * 10^{-19}

E(eV) = E(J)/ 1.602 x 10^{-19}

Photoelectric effect

In 1887, H. Hertz performed a very interesting experiment in which electrons (or electric current) were ejected when certain metals (for example potassium, rubidium, cesium, etc.) were exposed to a beam of light as shown in Fig.2.9.



The phenomenon is called the photoelectric effect.
The results observed in this experiment were:

- The photoelectric current is directly proportional to the light intensity.
- The kinetic energy of the photoelectrons is directly proportional to the light frequency.
- The threshold frequency varies with material, it is different for different materials.

For each metal, there is a characteristic minimum frequency, ν^o (also known as threshold frequency)
At a frequency $\nu > \nu^o$, the ejected electrons have a certain kinetic energy.
The kinetic energies of these electrons increase as the frequency of the light increases.
Einstein (1905) explained the photoelectric effect using Planck's quantum theory of electromagnetic radiation as a starting point.

Shining a beam of light onto a metal surface can therefore be viewed as shooting a beam of particles: photons. When a photon with sufficient energy strikes an electron in the metal atom, it transfers its energy instantaneously during the collision, ejecting the electron without any time lag. The greater the energy possessed by the photon, the greater the transfer of energy to the electron and the greater the kinetic energy of the ejected electron. In other words, the kinetic energy of the ejected electron is proportional to the frequency of the electromagnetic radiation. Since the striking photon has energy equal to $h\nu$ and the minimum energy required to eject the electron is $h\nu 0$ (also called the work function, W^o; Table 2.2).then the difference in energy ($h\nu - h\nu^o$) is transferred as the kinetic energy(E_K)of the photoelectron. According to the conservation of energy, the kinetic energy of the ejected electron is given by equation 2.7.

kinetic energy of ejected electron (E_K) = $E - E^o = h\nu - h\nu^o = h(\nu - \nu^o)$

When a metal is struck by light with energy above the threshold energy Eo, the number of emitted electrons is proportional to the intensity of the light beam, but the kinetic energy of the emitted electrons is proportional to the frequency of the light. Thus, Einstein showed that the energy of the

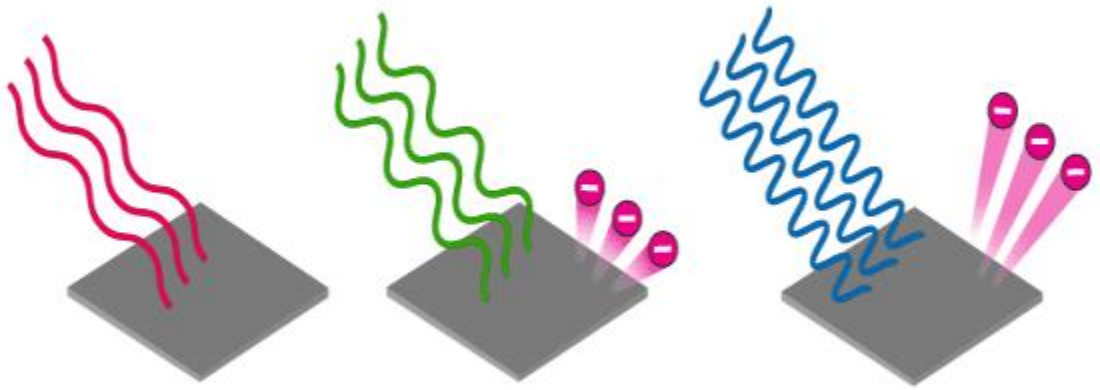
$$h\nu = h\nu^0 + \frac{1}{2} m v^2$$

where m_e is the mass of the electron and v is the velocity associated with the ejected electron. Lastly, a more intense beam of light consists of a larger number of photons; consequently, the number of electrons ejected is also larger as compared to that in an experiment in which a beam of weaker intensity of light is employed.

The phenomenon of metals releasing electrons when they are exposed to the light of the appropriate frequency is called photoelectric effect, and the electrons emitted during the process are called photoelectrons.

Note: Each photon carries a specific energy related to its wavelength, such that photons of short wavelength (blue light) carry more energy than long wavelength (red light) photons. To release an electron from a metal plate required a minimal energy which could only be transferred by a photon of energy equal or greater than that minimal threshold energy (i.e. the wavelength of the light had to be a sufficiently short). The photoelectric earned Einstein the Nobel Prize, and introduced the term ``photon" of light into our terminology.

Note: This effect is used in many devices, including TV, cameras, camcorders, and night vision viewers.



Note: Application of photoelectric phenomena is Photoelectron spectroscopy is a method used to determine work function of various elements. When monochromatic light of sufficient frequency shines on a metal plate.

Work function

Any object (including atoms) can emit or absorb only certain quantities of energy is quantized, it occurs in fixed quantities, rather than being continuous. Each fixed quantity of energy is called a quantum atom changes its energy state by emitting or absorbing one or more quanta of energy. Surface electrons are bound to metals with a small amount of energy. Some of the incident photons enter the surface, collide with atoms of the metal and are totally absorbed. They give their energy to an electron, which, if the absorbed energy was great enough, then break free from the atom. The photoelectric effect is the result of collisions between photons and electrons that knock the electrons out of the metal.

W = work function: the minimum energy which is required to remove an electron from the surface of given solid usually metals.

E photon = W° + E (kinetic energy) …..1

E= h υ ----2 $\omega° = ħυ°$……. 3

then substituted in (1)

$E_k = ħ\boldsymbol{υ} - W°$ …….4

$E_k = ½ mv^2$ ….. 5 substituted in (4) equation

$½ mv^2 = ħ\boldsymbol{υ} - W°$ ……6

υ=c/λ ….. 7

$½ mv^2 = hc/λ - hυ°$……8 hυ° = h

$c/λ – ½ mv^2$……9

$$\nu° = \frac{c}{\lambda} - \frac{mv^2}{2h}$$

Where υ° = threshold frequency

m= mass of electron

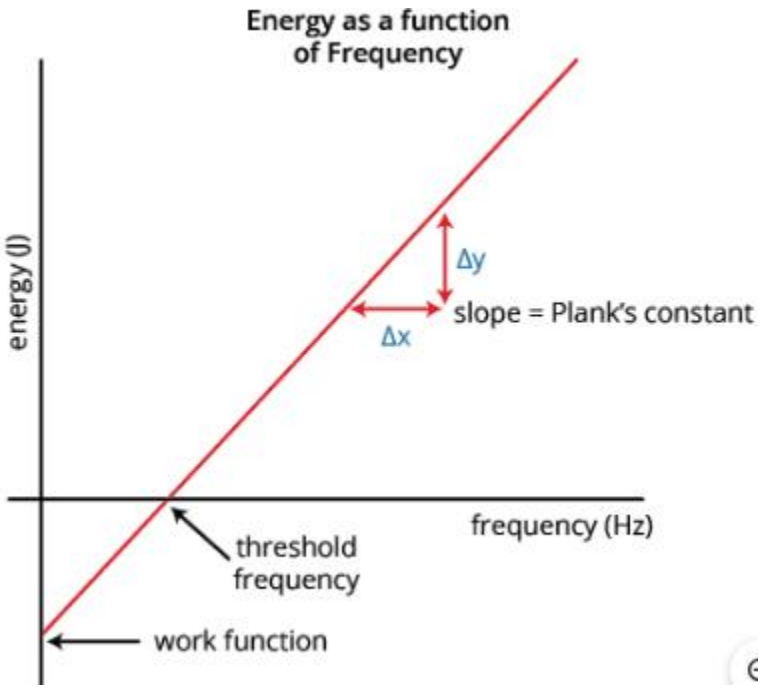
υ=speed of electron

Note

If E of photon < W° work function that means the electron could not move from metals

If E of the photon = W° the electron move from metal without generate current

If E of photon > W° the electron move from metal surface and generate current.



The relationship between the maximum kinetic energy of photoelectrons and the frequency of incident light is linear. The intercept on the frequency axis gives the threshold frequency. The number of emitted photoelectrons increases with intensity but emission only occurs if the frequency exceeds the threshold value.

Ex (1): When light of a wavelength of (125 nm) strikes certain metal, electrons having a velocity of (8.2×10^5 m/s) are emitted from the surface of the metal. What is the threshold frequency of the metal?

)

Note: J = Kg.m^2.s^{-2} = g. cm^2. S^{-2}

Ex (2): An experimenter finds that no photo electrons are emitted from tungsten unless the wavelength of light is less than (270 nm). However, in order to carry out her experiment she needs to produce photo electrons with a maximum kinetic energy Kmax =2.0 eV. What frequency of light should be used to illuminate the tungsten?

$$w^\circ = \hbar * \upsilon^\circ$$

$$w^\circ = \hbar * \frac{c}{\lambda}$$

$$w^\circ = \frac{(6.626 \times 10^{-34}\ J.S)(3 \times 10^{8} ms - 1)}{270 * 10^{-9}\ m} = \ 7.36 \times 10^{-19} J$$

Ekmax = 2.0* 1.6022*10^{-19} J = 3.2*10^{-19}J

E photon = 7.36 *10^{-19} + 3.2*10^{-19}J= 10.56*10^{-19} J

E= ħ*υ

υ = E/ħ

υ = 10.56*10^{-19} / 6.626*10^{-34}J.s

υ = 1.56*10^{15} s-1 or Hz

Black body radiation

The energy emitted by an object when it is heated. The wavelength of energy emitted by an object depends on only its temperature, not its surface or composition. Hence an electric stove burner or the filament of a space heater glows dull red or orange when heated, whereas the much hotter tungsten wire in an incandescent light bulb gives off a yellowish light.

The intensity of radiation is a measure of the energy emitted per unit area. A plot of the intensity of blackbody radiation as a function of wavelength for an object at various temperatures is shown in Figure 6.6. For example, classical physics predicted that as wavelength decreased, the intensity of the radiation an object emits should increase in a smooth curve without limit at all temperatures, as shown by the broken line for 6000 K. Thus, classical physics could not explain the sharp decrease in the intensity of radiation emitted at shorter wavelengths. The German physicist Max Planck (1858–1947) explained the ultraviolet catastrophe by proposing that the energy of electromagnetic waves is quantized rather than continuous. This means that for each temperature, there is a maximum intensity of radiation that is emitted in a blackbody object, corresponding to the peaks in Figure 6.6, so the intensity does not follow a smooth curve as the temperature increases, as predicted by classical physics. Thus, energy could be gained or lost only in integral multiples of some smallest unit of energy, a quantum.

A black body is a body that absorbs all the EM radiation (light ...) that strikes it. To stay in thermal equilibrium, the radiation must emit at the same rate as its absorption in order for the black body to radiate well.

Blackbody Radiation: It is known that the amount of radiation energy emitted from a surface at a given wavelength depends on the material of the body and the condition of its surface as well as the surface temperature. **A black body** a material or substance completely absorbs all frequencies of light. Because of the laws of thermodynamics, this ideal body must also re-emit as much light as it absorbs. If we heat an object up to about 1500 degrees, we will begin to see a dull red glow and we say the object is red hot. If we heat something up to about 5000 degrees, near the temperature of the sun's surface, it radiates well throughout the visible spectrum and we say it is white-hot. A solid object emits visible light when it is heated to about 1000 K. This is called blackbody radiation. The color of (and the intensity) the light changes as the temperature changes. Color is related to wavelength and frequency, while temperature is related to energy**.** Figure 7

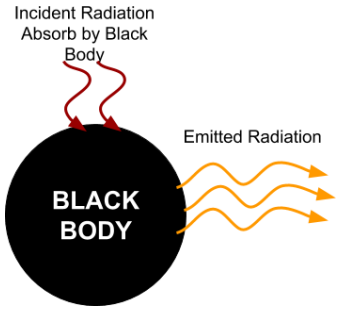
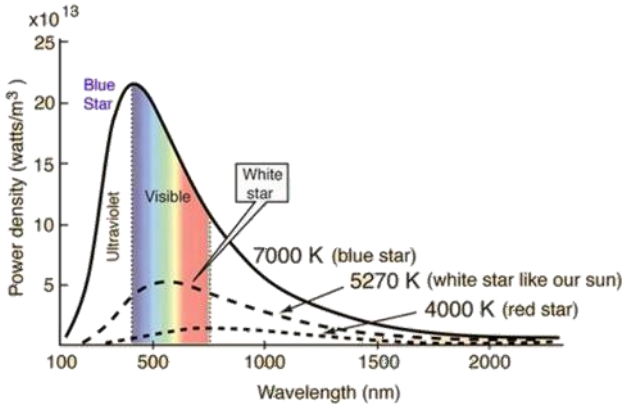


Figure 7: show the black body radiation

Wien's displacement law

When the temperature of a blackbody radiator increases, the overall radiated energy increases and the peak of the radiation curve moves to shorter wavelengths. When the maximum is evaluated from the Planck radiation formula, the product of the peak wavelength and the temperature is found to be a constant. This cure show that temperature proportion inverse with wavelength. This relationship is called Wien's displacement law and is useful for determining the temperatures of hot radiant objects such as stars, and indeed for a determination of the temperature of any radiant object whose temperature is far above that of its surroundings.



$$\lambda_M T = 2.90 \times 10^{-3}\, m.K \qquad \text{Wien's displacement law} \quad \ldots\ldots 14$$

Where, λ_{max} = Wavelength of maximum intensity in meters,

T = Temperature of the black body in kelvins

If temperature is rises, peak of become higher and λ shift to the shorter wavelength yellow light has shorter wavelength than red light, body that glows yellow hotter and brighter than one of the same sizes that glow red.

Stefan-Boltzmann law: The total energy E radiated from per unit surface area (square meter) of black surface is proportional to the fourth power of the absolute temperature (T4). Eq. (15).

$$J = \sigma \varepsilon A T^4 \quad \ldots\ldots 15$$

Where J * = power radiated (Watt) per unit area from black body.

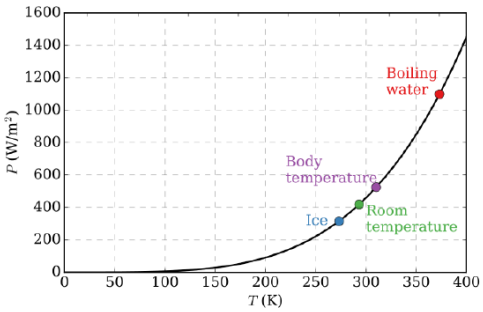
e = Emissivity = 1 for ideal radiator

σ = Stefan-Boltzmann constant =5.67*10^{-8} W.m^{-2}. K^{-4}.

A = Surface area (m^2)

T= surface temperature of the body in K.

Emissivity: Is the ratio of energy radiated by the body to the energy radiated by a black body with the same temperature.



Bohr's theory of the atom

Bohr's model is shown in Figure 3.1. An electron of charge –*e* and mass (m) move around a heavy nucleus of charge +*e*. ordinarily the electron would move in a straight line, but the attraction of the nucleus bends its path so that it moves with a constant velocity v in a perfect circle of radius *r* around the nucleus. The situation and the mathematics are very similar to that of a planet arcing round the sun. The major difference is that instead of the force of gravity there is an electrostatic force of attraction FE between the proton and the electron described by coulomb' law:

$$F_{coulomic} = \frac{-ze^2}{r^2} \quad \cdots 1$$

The movement of an electron in its orbit would create a centrifugal force, which gives it a tendency to fly away from the nucleus. This force is given by

$$F_{centrifugal} = \frac{mv^2}{r} \quad \cdots 2$$

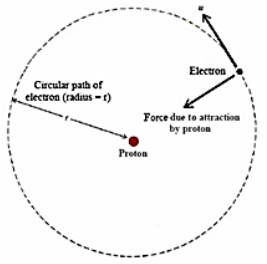


Figure 3.1: Electron movement

In order to calculate the radius of orbit by this equation

$$r = \frac{n^2\, h^2}{4\pi^2 mze^2}$$

Assumption of Bohr's theory

1. The H atom has only certain energy levels, which Bohr called stationary states. Each state is associated with a fixed circular orbit of the electron around the nucleus. The higher the energy level, the farther the orbit is from the nucleus.
2. The atom does not radiate energy while in one of its stationary states. Even though it violates principles of classical physics, the atom does not change energy while the electron moves within an orbit.
3. The atom changes to another stationary state (the electron moves to another orbit) only by absorbing or emitting a photon.

Ex: use the Bohr's theory to calculate the first orbit radius of hydrogen atom.

$Z_H = 1$, $Z_{He} = 2$, $Z_{Li} = 3$

$$r = \frac{n^2\, h^2}{4\pi^2 mze^2}$$

$$r = \frac{1^2\ (6.626 \times 10^{-27} erg.s)^2}{4(3.14)^2(9.1 \times 10^{-28} g)(1)(4.8 \times 10^{-10} e.s.u)^2}$$

$$e.s.u = \ erg^{1/2} cm^{1/2}.$$

$r = 0.529 \times 10^{-8}$ cm

for another orbit you can use this equation

$$r = a° \times n^2$$

Ex: use the Bohr's theory to calculate the first, second and third orbit radius for hydrogen atom.

$$\boldsymbol{r = \frac{n^2\, h^2}{4\pi^2 mze^2}}$$

r = 0.529×10^{-8} cm as mention in previous example

$r_n = a° \times n^2$

$r_2 = 0.529\times10^{-8}$ cm $\times (2)^2 = 2.11\times10^{-8}$ cm for second orbit

$r_3 = 0.529\times10^{-8}$ cm $\times (3)^2 = 4.761\times10^{-8}$ cm for third orbit

for another atom like He^+, you can calculate the radius in first, second orbit and third.

$$\boldsymbol{r_{He} = \frac{a°n^2}{z} = \frac{0.529 \times 10^{-8} \times (1)^2}{2}} = 0.2645 \times 10^{-8} cm$$

$$\boldsymbol{r_{He} = \frac{a°n^2}{z} = \frac{0.529 \times 10^{-8} \times (2)^2}{2}} = 1.058 \times 10^{-8} cm$$

The same calculation can do it for Li^{+2} as He^+ to calculate the first and second orbit except use z= 3 (atomic number for Li)

Ex: the radius of innermost electron orbit of the hydrogen atom is 5.3×10^{-11}. what are the radii of the n = 2 and n =3 orbit?

n = 2 → $r = a°\times n^2$

$r = 5.3 \times 10^{-11} (2)^2 \rightarrow r = 2.12 \times 10^{-10}$m

Where n= 3

$r = 5.3 \times 10^{-11} (3)^2$

$r = 4.77\times 10^{-10}$m

The velocity of electron

$$V = \frac{h}{2\pi m a^{\circ} n}$$

a = 0.529×10^{-8}cm for hydrogen

Unit of speed = $m.s^{-1}$

ex: use the Bohr's theory to calculate the velocity of electron in the first, second and third orbit for hydrogen atom.(h.w)

Note: J= Kg. $m^2.s^{-1}$ Erg = $g.cm^2.s^{-1}$

This equation below used for other atoms like He and Li

$$V_n = \frac{V1}{n}$$

Energy of an Electron in Hydrogen Atom

The energy of an electron moving in one particular energy level of the hydrogen atom in the Bohr models can be calculated by the total energy or the sum of the kinetic energy and the potential energy of an electron in physics and chemical science.

Here **kinetic energy = ½ mv^2**

and **potential energy for moving electron = $e^2/2r$.**

The total energy for the nth level of the hydrogen atom in Bohr model,

$$E = \frac{-Ze^2}{2a^{\circ}n^2}$$

$$E_n = \frac{E1}{n^2}$$

where E_1 = energy of the first orbit of the hydrogen atom in the Bohr model. As the principal quantum number (n) increases the energy becomes less negative and hence the Bohr system becomes less stable. so E1<E2<E3

NOTE: The Bohr's model of hydrogen atom applicable to the species H, He^{+}, Li^{+2} contain one electron

EX: use the Borh's theory to calculate the energy of electron in first, second and third orbit for hydrogen atom.

$$\boldsymbol{E = \frac{-Ze^2}{2a^{\circ}n^2}} = \frac{-(1))(4.8 \times 10^{-10} e.s.u)^2}{2(0.529 \times 10^{-8} cm)1^2} = 4.53 \times 10^{-2}\, erg$$

NOTE: $\mathrm{E} = \frac{(e.s.u)^2}{cm} = \frac{erg.cm}{cm} = \mathrm{erg}$

Limitations of Bohr's Theory

Bohr's biggest contribution in his model was to introduce quantum principles to classical physics, but his model had a few limitations:

1- Spectra of Large atoms; The Bohr model could only successfully explain the hydrogen spectrum. IT could NOT accurately calculate the spectral lines of larger atoms. The model only worked for hydrogen-like atoms, if the atom had only one electron.

2- Relative Spectra Intensity; Bohr's model could not explain why the intensity of the spectra lines were NOT all equal.

3- Hyperfine spectral lines; with better equipment and careful observation, it was found that there were previously undiscovered spectral lines. These were named hyperfine lines and they accompanied the other more visible lines. Bohr's model could not explain why this was the case due to the lack of equipment and development in quantum physics.

4- The Zeeman Effect; It was found that, when hydrogen gas was excited in a magnetic field, the produced emission spectrum was split. Bohr's model could not account for this. Solved by accounting for the existence of a tiny magnetic moment of each electron.

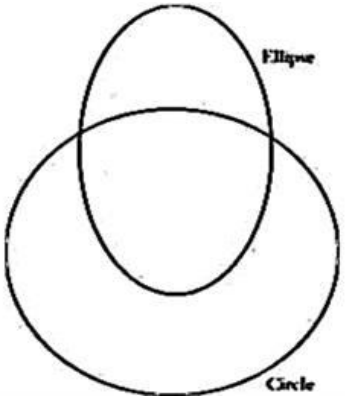
5-Heisenberg's uncertainty principle: According to Borh's model, electron move around the nucleus in a well-defined orbit and hence its position and moment can be determined simultaneously. But that's impossible and against the Heisenberg's uncertainty principle (It is impossible to determine simultaneously the exact position and moment of a small moving particle like an electron).

6-According to Bohr, the radiation results when an electron jumps from one energy orbit to another energy orbit, but how this radiation occurs is not explained by Bohr.

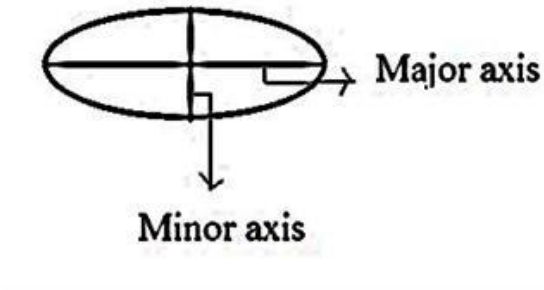
Sommerfeld atomic model

This model explains the fine spectrum of Hydrogen atom. The important postulates of Sommerfeld atomic model are

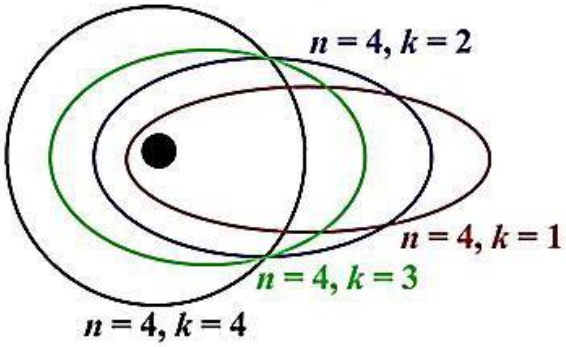
1- The orbits may be both circular and elliptical.



2- When path is elliptical, then there are two axis – major axis & minor axis. When length of major & minor axis becomes equal then orbit is circular.



3- The angular momentum of electron moving in an elliptical orbit is (kh/2π). Where k is an integer except zero. Value of k = 1, 2,3,4….. . (n/k) = length of major axis / length of minor axis. With increase in value of k, ellipticity of the orbit decreases. When n= k, then orbit is circular.



4- Sommerfeld suggested that orbits are made up of sub energy levels. These are s,p,d,f. These sub shells possess slightly different energies. Bohr gave a quantum number 'n', which determines the energy of electron. Sommerfeld introduced a new quantum number called Orbital or Azimuthal Quantum number

(l) which determines the orbital angular momentum of electron. Values of l =0 to (n-1)

For, n=1 ; l=0 ; 1s sub shell

n=2 ; l=0,1 ; 2s , 2p sub shell

n=3 ; l=0,1 ,2 ; 3s , 3p , 3d sub shell

n=4 ; l=0, 1, 2 , 3 ; 4s , 4p , 4d , 4f sub shell

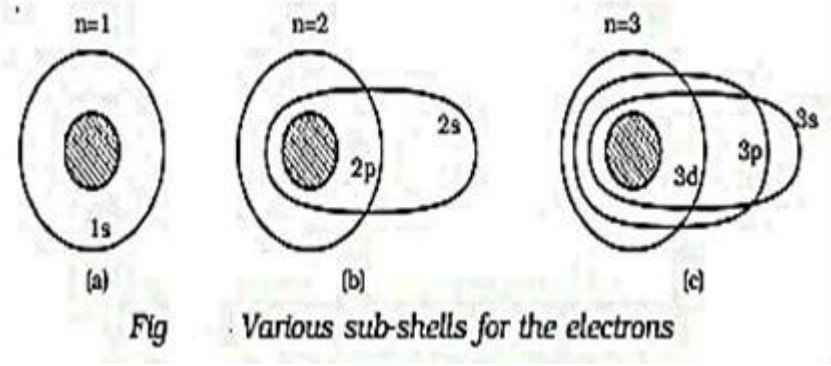


Fig Various sub-shells for the electrons

5- When an electron jumps from one orbit to another orbit, the difference of energy (ΔE) depends upon sub energy levels.

6- It explains the splitting of individual spectral lines of hydrogen & thus fine spectrum . It could not predict the exact number of lines which are actually present in the fine spectrum.

Defects of Sommerfeld atomic model

1- This model does not explain the behavior of system having more than one electron.
2- This model does not explain the Zeeman & Stark effect.

Wave Mechanics

DeBroglie suggested that particles of matter such as electrons have some properties of waves. If electrons were wave like and restricted to orbits of fixed radii, only certain possible frequencies and energies would be allowed. From mass-energy equivalence**.**

$$E = mv^2$$

and the equation for the energy of a photon

$$E = hv = \frac{hc}{\lambda}$$

De Broglie derived:

$$\boldsymbol{mv^2 = \frac{hc}{\lambda}}$$

$\boldsymbol{\lambda = \frac{hc}{mv^2}}$ as v = c

$$\boldsymbol{\lambda = \frac{h}{mv}}$$

Where λ is De Broglie wavelength, m is the mass and v is the velocity

An object's wavelength is inversely proportional to its mass; heavy objects have wavelengths that are very much smaller than the object. Fast moving electrons have wavelengths close to the size of an atom (~10 –10 m).

Ex: Determine the DeBroglie wavelength of an electron moving at the speed of light

$$\boldsymbol{\lambda = \frac{h}{mv}}$$

$$\boldsymbol{\lambda = \frac{6.626 \times 10^{-34} J.s}{9.1 \times 10^{-31} Kg \times 3 \times 10^{8} ms^{-1}}}$$

$$\frac{J.s}{Kg.m.s^{-1}} = \frac{Kg.m^2.s^{-2}.s}{Kg.m.s^{-1}} = m$$

Note: v = c = 3×10^8 ms^{-1}

Ex: Determine the DeBroglie wavelength of an electron moving at one tenth the speed of light.

One tenth = 1/10 = 0.1

V= $3\times10^8\times0.1$

$$\lambda = \frac{h}{mv}$$

$$\lambda = \frac{6.626\times10^{-34}J.s}{9.1\times10^{-31}Kg\times3\times10^8\times0.1\ ms^{-1}} = \text{---- m}$$

Quantum mechanics (wave mechanics)

• Does not allow us to specify exact location of electrons, we can predict high probability of finding an electron

• Use the term atomic orbital instead of "orbit" to describe the electron's position within the atom.

Heisenberg's Uncertainty Principle

States (that it is impossible to know both the position and momentum of a moving particle at the same time). It is stated mathematically,

$\Delta x\ \Delta p \geq h/4\pi$

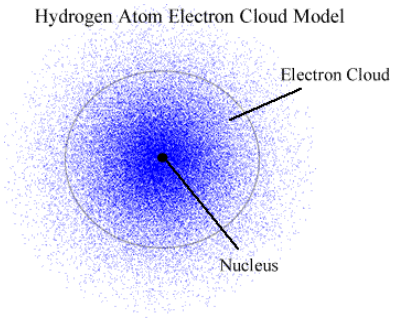
Where Δx and Δp are the uncertainties in measuring the position and momentum. Applying Heisenberg uncertainty principle to the H atom, we see that in reality the electron does not in orbit the nucleus in a well-defined path, as Bohr thought.

Schrodinger wave mechanics

In 1927 Erwin Schrodinger (Austrian physicist) used a complicated mathematical technique formulated an equation that describes the behavior and energies of submicroscopic particles. In general the Schrodinger equation requires advanced calculus to solve and it is important to know that the equation incorporates both particles behavior in terms of mass, m and wave behavior in terms of wave function Ψ (psi), which depends on the location in space of the system. According to wave theory, the intensity of light is proportional to the square of the amplitude of the wave or

Ψ^2. The most likely to find a photon is where the intensity is greatest, that is, where the value of Ψ^2 is greatest. Schrodinger wave equation E=HΨ) began a new area in physics and chemistry called the quantum mechanics (wave mechanics).

- Quantum Mechanical Model
- Discovered the regions of probability for locating electrons
- Discovered the regions known as electron clouds
- Mathematical explanations for the location of electrons, every electron has four quantum numbers**.**



The energy difference between any two energy levels is given by:

$$\boldsymbol{E = -2.18 \times 10^{-18}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)}$$

Ex: A hydrogen atom absorbs a photon of UV light, and its electron enters the n = 4 energy level. Calculate (a) the change in energy of the atom and (b) the wavelength (in nm) of the photon.

a) $\boldsymbol{\Delta E = -2.18 \times 10^{-18}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)}$

$$\boldsymbol{\Delta E = -2.18 \times 10^{-18}\left(\frac{1}{4^2} - \frac{1}{1^2}\right)}$$

$$\boldsymbol{\Delta E = -2.18 \times 10^{-18}\left(\frac{1}{16} - \frac{1}{1}\right) = 2.04 \times 10^{-18}\, J}$$

b)

Inorganic Chemistry

Dr.Sarab Alazawi **2026-2027** **first year**

$$\Delta E = h\nu = \frac{hc}{\lambda}$$

$$\lambda = \frac{hc}{\Delta E} = \frac{6.626\times10^{-34} J.s \times 3\times10^{8} ms-1}{2.04\times10^{-18} J} = 9.74\times10^{-8} m = 9.74\times10^{-8}\times\frac{1nm}{10^{-9}} = 97.4 \ nm$$

Quantum Number

In quantum mechanics, three quantum numbers are required to describe the distribution of electrons in atoms. These numbers are derived from the mathematical solution of the Schrodinger equation for the hydrogen atom.

1- *The* ***principal quantum number (n)*** tells the average relative distance of an electron from the nucleus, and the energy of the electron in an atom. (It can have only positive integer ***n***= 1,2,3,4,…..). The larger the value of ***n***, the higher energy and the larger orbital, or electron shell.

2- The ***angular momentum quantum number (ℓ)*** *or* ***orbital quantum number*** describes the ***shape*** of the orbital, and the shape is limited by the principal quantum number ***n*** (the shape of the region of space occupied by the electron), (***ℓ= 0, 1, 2, 3, …… n-1***).

* ***Notice***; the value of ***ℓ*** defines the shape of the orbital, and the value of ***n*** defines the size.

* ***Notice*****; Orbitals** that have the **same** value of ***n*** but **different** values of ***ℓ*** are called ***subshells***. These subshells are given different letters to help chemists distinguish them from each other.

*For example ***ℓ= 0, 1, 2, 3***

Name = ***s, p, d, f***

1- The ***magnetic quantum number ($m_ℓ$)*** represents the *orientation of the region in space occupied by an electron with respect to an applied magnetic field.* (The value of $m_ℓ$ depends on the value of ***ℓ, $m_ℓ$= +l , 0 , -l***).

4- Spin quantum number

According to electromagnetic theory, a spinning charge generates a magnetic field, and it is this motion that causes an electron to behave like a magnet. The following figure shows the two possible spinning motions of an electron, one clockwise and the other counter clockwise. Only two values are allowed for m_s +1/2 and -1/2.

Atomic Orbitals

The following table shows the relation between permissible quantum numbers and atomic orbital's. We see that when $\ell = 0$, $(2\ell + 1) = 1$ and there is only one value of ml, thus we have an s orbital. When $\ell = 1$, $(2\ell + 1) = 3$, so there are three values of ml or three p orbital's, labeled px, py and pz. When $\ell = 2$, $(2\ell + 1) = 5$ and there are five values of ml, and the corresponding five d orbital's are labeled with more elaborate subscripts.

Quantum Numbers and Energy Levels

The energy states and orbitals of the atom are described with specific terms and are associated with one or more quantum numbers:

1. Level. The atom's energy levels, or shells, are given by the n value: the smaller the n value, the lower the energy level and the greater the probability that the electron is closer to the nucleus.

2. Sublevel. The atom's levels are divided into sublevels, or subshells, that are given by the ℓ value. Each designates the orbital shape with a letter:

ℓ = 0 is an s sublevel.

ℓ= 1 is a p sublevel.

ℓ= 2 is a d sublevel.

ℓ = 3 is an f sublevel

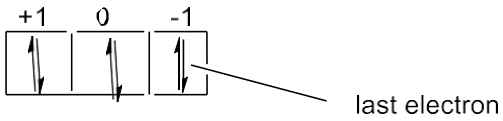
Ex: Give the name, magnetic quantum numbers, and number of orbitals for each sublevel with the given n and ℓ quantum numbers: (a) n = 3, ℓ = 2 (b) n = 2, ℓ= 0 (c) n = 5, ℓ = 1 (d) n = 4, ℓ = 3

Solution:

	n	ℓ	Subshell name	Possible ml	No.of orbtal
a	**3**	**2**	**3d**	**+2,+1.0.-1, -2,**	**5**
b	**2**	**0**	**2s**	**0**	**1**
c	**5**	**1**	**5p**	**+1,0,-1**	**3**
d	**4**	**3**	**4f**	**+3, ,+2, +1,0,-1, - 2.-3,**	**7**

Ex: Write a set of quantum numbers for the last electrons in ground state and ions in a Ne atom.

$_{10}Ne = 1s^2\ 2s^2\ 2p^6$



$n = 2, \ell = 1, m\ell = -1, m_s = -1/2$

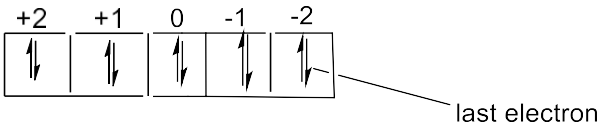
***no ions for noble gas**

Ex: Give the value for all four quantum number for the last electron in the ground state of Cu29.

Cu_{29} : $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^9$

Cu_{29} : $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1 3d^{10}$

n= 3, ℓ= 2, mℓ = -2, ms= -1/2



Q: write the complete set quantum number that represent valence electron $_6C$?

$_6C$ $1s^2$ $2s^2$ $2p^2$

E1: n= 2, ℓ=0 , mℓ= 0 ms= +1/2

E2: n= 2, ℓ=0 , mℓ= 0 ms= -1/2

E3: n= 2, ℓ=1 , mℓ= +1 ms= +1/2

E4: n= 2, ℓ=1 , mℓ= 0 ms= +1/2

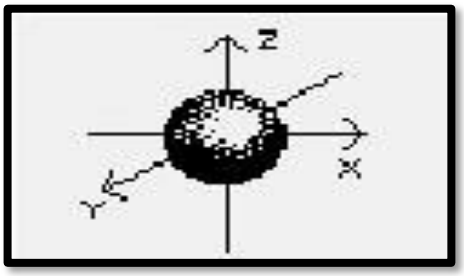
Atomic Orbital Shapes

Size of orbitals; defined as the surface that contains 90% of the total electron probability.

*S Orbital

S orbitals are spherical with the nucleus at the center. When ***n*** increases, **s** orbitals become larger and higher in energy because of their increased distance from the nucleus.

Note: Each subshell of the H atom has orbitals with a characteristic shape. s orbitals ($\ell = 0$) are spherically symmetrical around the nucleus.

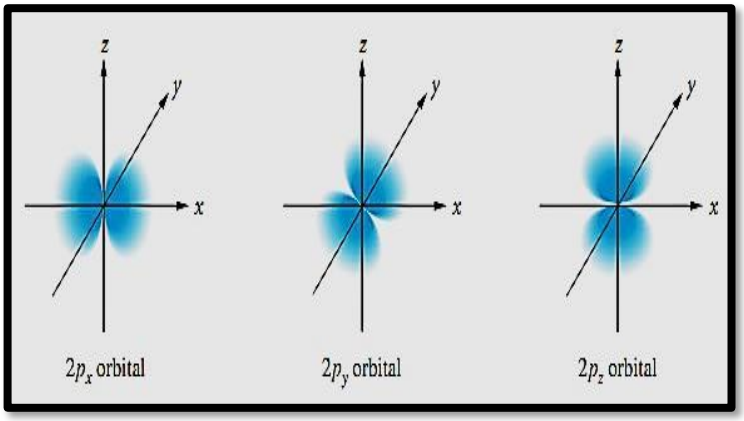


P Orbitals

There are three **P** orbitals in each **P** subshell, occur in levels ***n***=2 and greater. All **P** orbitals have the same basic shape (two lobes arranged along a straight line with the nucleus between the lobes) but differ in their orientations in space). We denote these orbitals as $\mathbf{2P_x}$, $\mathbf{2P_y}$, and $\mathbf{2P_z}$. A $\mathbf{2P_x}$ orbital has its greatest electron probability along the **x-axis**, a $\mathbf{2P_y}$ orbital along the **y-axis**, and a $\mathbf{2P_z}$ orbital along the **z-axis**.

Notice; as the value of ***l*** increases, the number of orbitals in a given subshell increases, and the shapes of the orbitals become more complex.

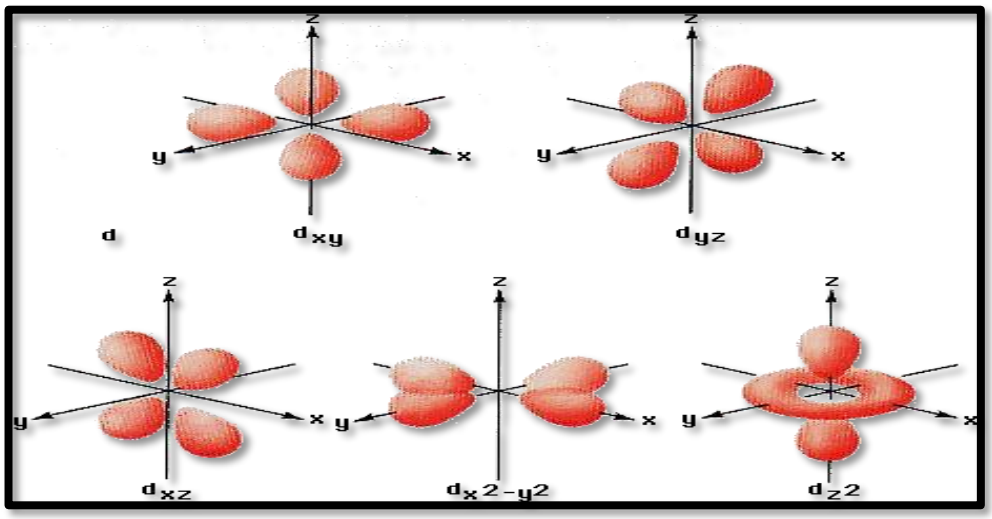
Energies of p orbitals: 2p < 3p < 4p.



d Orbitals

Occur in levels ***n*** = 3 and greater. Two fundamental shapes;

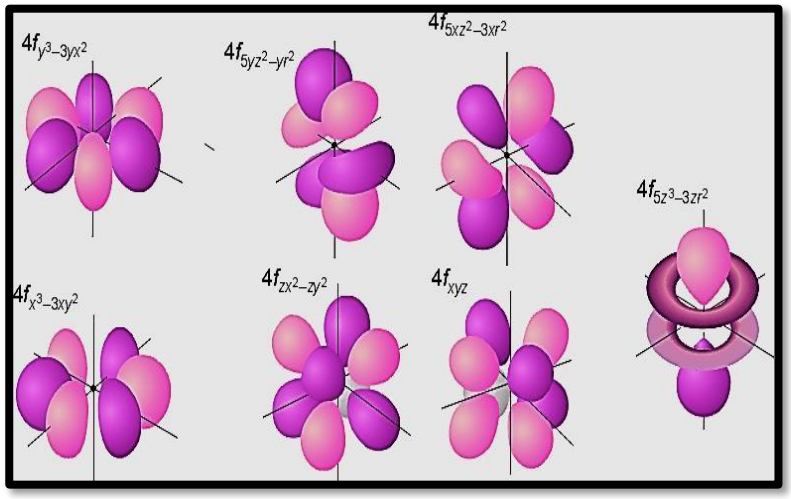
- ***a.*** Four orbitals with four lobes for each one, centered in the plane indicated in the orbital label **dxz**, **dyz**, **dxy**, and **$dx^2 - y^2$**
- ***b.*** Fifth orbital is uniquely shaped - **two lobes** along the **z-axis** and a **belt** centered in the **xy** plane **dz^2**.



f Orbitals Occur in levels ***n*=4** and greater, not involved in bonding in most compounds. Principal shells with ***n*** = 4 can have subshells with ***l*** = **3** and m_l values of **+1**, **+2**, **+,. −1, −2**, and**−3**. These subshells consist of seven f orbitals. Each f orbital has three nodal surfaces, so their shapes are complex.

Inorganic Chemistry

Dr.Sarab Alazawi **2026-2027** **first year**



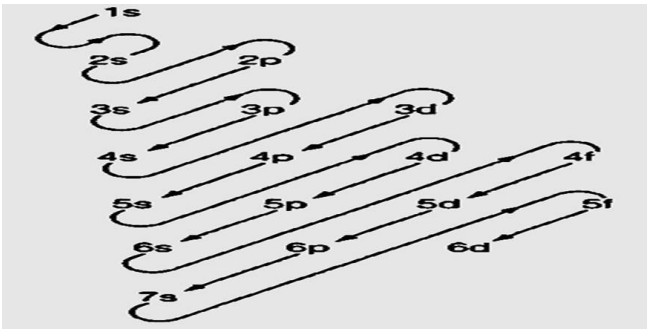
Electron Configurations

The energy of an electron depends on the type of orbital that it occupies. Orbitals with the same energy level are called ***degenerate orbitals***. The order in which the orbitals are filled by electrons is determined by just three simple principles:

1- The ***Aufbau*** (or ***Building up***) principle. The lowest-energy orbital is filled first.

2- The Pauli Exclusion Principle. Each orbital can accommodate a maximum of two electrons that have opposite spin states.

3-Hund's Rule. When dealing with degenerate orbitals, such as p orbitals, one electron is placed in each degenerate orbital first, before electrons are paired up.



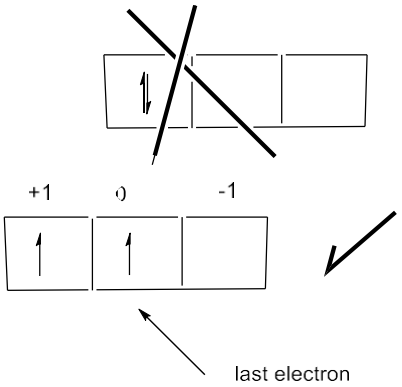
* The next tables represent the electronic configuration of Atoms.

Inorganic Chemistry

Dr.Sarab Alazawi **2026-2027** **first year**

Z	Symbol	Configuration	Z	Symbol	Configuration
1	H	$1s^1$	56	Ba	(Xe) $6s^2$
2	He	$1s^2$	57	La	(Xe) $5d^1\ 6s^2$
3	Li	$1s^2\ 2s^1$	58	Ce	(Xe) $4f^2\ 6s^2$
4	Be	$1s^2\ 2s^2$	59	Pr	(Xe) $4f^3\ 6s^2$
5	B	$1s^2\ 2s^2\ 2p^1$	60	Nd	(Xe) $4f^4\ 6s^2$
6	C	$1s^2\ 2s^2\ 2p^2$	61	Pm	(Xe) $4f^5\ 6s^2$
7	N	$1s^2\ 2s^2\ 2p^3$	62	Sm	(Xe) $4f^6\ 6s^2$
8	O	$1s^2\ 2s^2\ 2p^4$	63	Eu	(Xe) $4f^7\ 6s^2$
9	F	$1s^2\ 2s^2\ 2p^5$	64	Gd	(Xe) $4f^7\ 5d^1\ 6s^2$
10	Ne	$1s^2\ 2s^2\ 2p^6$	65	Tb	(Xe) $4f^9\ 6s^2$
11	Na	(Ne) $3s^1$	66	Dy	(Xe) $4f^{11}\ 6s^2$
12	Mg	(Ne) $3s^2$	67	Ho	(Xe) $4f^{11}\ 6s^2$
13	Al	(Ne) $3s^2\ 3p^1$	68	Er	(Xe) $4f^{12}\ 6s^2$
14	Si	(Ne) $3s^2\ 3p^2$	69	Tm	(Xe) $4f^{13}\ 6s^2$
15	P	(Ne) $3s^2\ 3p^3$	70	Yb	(Xe) $4f^{14}\ 6s^2$
16	S	(Ne) $3s^2\ 3p^4$	71	Lu	(Xe) $4f^{14}\ 5d^1\ 6s^2$
17	Cl	(Ne) $3s^2\ 3p^5$	72	Hf	(Xe) $4f^{14}\ 5d^2\ 6s^2$

Ex: determine the four set of quantum number for the last electron in the following atoms $_6C$, $_{12}Mg$, $_{23}V$



Solution:

1- Write the electron configuration

$_6C$: $1s^2\ 2s^2\ 2p^2$

2- last electron in orbital p

n = 2, ℓ= 1 , mℓ= 0, ms = +1/2

Note: The 4s orbital is slightly lower in energy than the 3d and fills first. In any period, the ns sublevel fills before the (n - 1)d sublevel. Other variations in the filling pattern occur at higher values of n because sublevel energies become very close together.

Categories of Electrons

There are three categories of electrons:

1. **Inner (core):** electrons are those an atom has in common with the previous noble gas and any completed transition series. They fill all the lower energy levels of an atom.
2. **Outer electrons**: are those in the highest energy level (highest n value). They spend most of their time farthest from the nucleus.
3. **Valence electrons**: are those involved in forming compounds:

For main-group elements, the valence electrons are the outer electrons.

For transition elements, in addition to the outer ns electrons, the (n - 1)d electrons are also valence electrons, though the metals Fe (Z = 26) through Zn (Z = 30) may use only a few, if any, of their d electrons in bonding.

The relation between main energy level and sublevel energy:

1- Main energy level

Each principal energy level can contain up to $2n^2$ electrons, where n is the number of the level. Thus, the first level can contain 2 electrons, $2(1^2) = 2$; the second 8 electrons, $2(2^2) = 8$; the third up to 18, $2(3^2) = 18$; and so on. Only seven energy levels are needed to contain all the electrons in an atom of any of those elements now known.

1- No. of electron = $2n^2$

2- **Sublevel energy** a- No. of electron = 2(2ℓ+1)

In s ℓ= 0 2(2(0)+1) = 2 electron

b- No. of electron in p sublevel

in p ℓ=1 2(2(1)+1)= 6 electron

3- Find the orbital in each sublevel

No. of orbital = (2ℓ+1)

In s sublevel ℓ= 0

No. of orbital = 2(0) +1= 1 orbital

4- Find the highest energy by n+ℓ

The (relative) energies of the orbitals can be predicted by the sum of n +ℓ for each orbital, according to the following rules:

a. Orbitals are filled in order of increasing (n + ℓ), which represents the relative energy.

b. If two orbitals have the same value of (n + ℓ), they are filled in order of increasing n.

Which one is the highest energy for the following?

1- 3d, 4s

2- 5s, 4p

Solution:

1- 3d n+ℓ= 3+2= 5

4s 4+0= 4

So energy of 3d > 4s

2- 5s n+ℓ= 5+0= 5

4p n+ℓ= 4+1= 5

5s > 4p (choose high value for n)

The Periodic Table

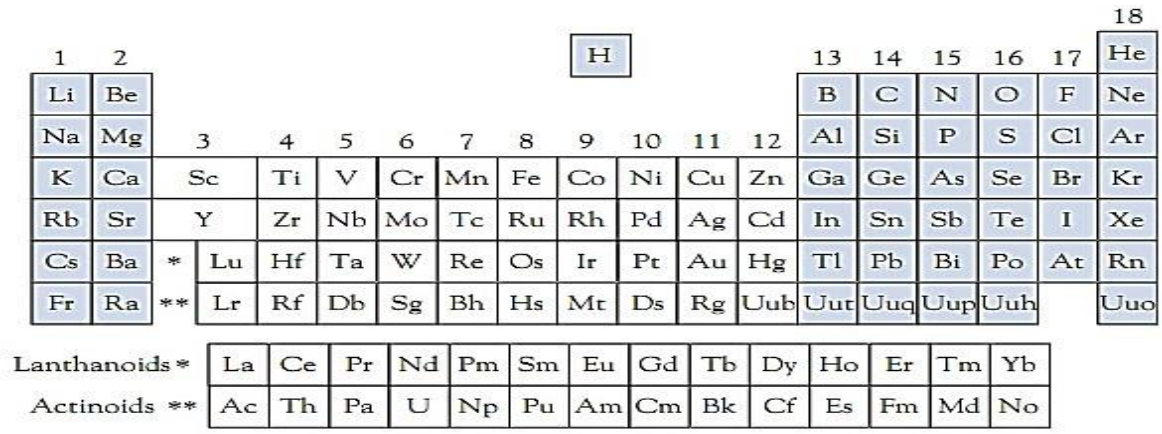
The idea of arranging the elements into a periodic table had been considered by many chemists, but either the data to support the idea were insufficient or the classification scheme was incomplete. **Mendeleev** and **Meyer** organized the elements in order of atomic weight and then identified families of elements with similar properties.

By arranging these families in rows or columns, and by considering similarities in chemical behavior as well as atomic weight, Mendeleev found vacancies in the table and was not able to predict the properties of several elements (***Gallium, Scandium, Germanium, Polonium***) that had not yet been discovered. When these predictions provide accurate, the concept of a periodic table was quickly established.

The discovery of additional elements not known in **Mendeleev's** time and the synthesis of heavy elements have led to the more complete modern periodic table. In the modern periodic table, a ***horizontal row*** of elements is called a ***period***, and a ***vertical column*** is a ***group*** or ***family***.

Inorganic Chemistry

Dr.Sarab Alazawi **2026-2027** **first year**



	1	2		3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
										H									He
	Li	Be												B	C	N	O	F	Ne
	Na	Mg												Al	Si	P	S	Cl	Ar
	K	Ca		Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
	Rb	Sr		Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
	Cs	Ba	*	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
	Fr	Ra	**	Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Uub	Uut	Uuq	Uup	Uuh		Uuo
Lanthanoids *				La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb		
Actinoids **				Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No		

Class of periodic elements: Based on electronic configuration

S – Block elements Group

1 (IA) and group 2 (IIA) which have ns^1 and ns^2 outermost electronic configuration belongs to the s-block elements. They are all reactive metals with low ionization energies, readily forms +1 and +2 ion respectively. Because of high reactivity they are never found pure form in nature.

p - block elements

The p-block elements comprise those belonging to group 13-18 and these together with the s-block elements (except noble gases) are called representative or main group elements. The outer most electronic configuration varies from ns^1 np^1 to ns2 np6 in each period. At the end of each period placed a noble gas element. Proceeding the noble gas family are two chemically important groups of non-metals. They are the halogens group (17) and the chalcogens (group 16). The non-metallic character increases as we move from left to right across a period and metallic character increases as we go down the group.

d – block elements

These are the elements of group 3 - 12 in the center of the periodic table. These elements have the general outer electronic configuration $(n-1)d^1$ to 10 ns^0 to 2. They are all metals. Transition metals form a bridge between the chemically active metals of s-block elements and the less active elements of groups 13 - 14.

f - block elements

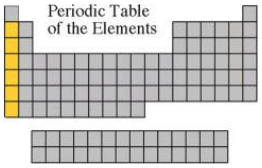
The two rows of elements at the bottom of the periodic table, called lanthanides (58Ce – 71Lu) and actinides (90Th – 103Lr) are characterized by the outer electronic configuration (n-2)f1 to 14 (n1) d0 – 1 ns2 . The last electron added to each element is filled in f – orbital. These two series

of elements are hence called the inner transition elements (f-block elements).They are also metals. Actinide elements are radioactive. Many of the actinide elements have been made only in nanogram or even less by nuclear reactions and their chemistry is not fully explored. The elements after uranium are called trans-uranium elements,

Classifications of the Elements

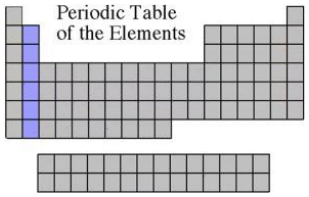
Alkali Metals

The alkali family is found in the first column of the periodic table. Atoms of the alkali metals have a single electron in their outermost level, in other words, 1 valence electron. They are shiny, have the consistency of clay, and are easily cut with a knife. They are the most reactive metals. They react violently with water. Alkali metals are never found as free elements in nature. They are always bonded with another element



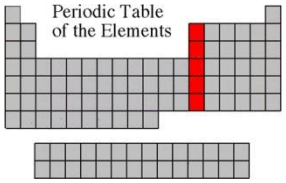
Alkaline Earth Metals

They are never found uncombined in nature. They have two valence electrons. Alkaline earth metals include magnesium and calcium, among others.



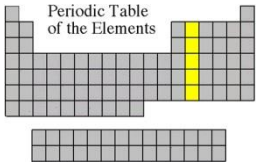
Metalloid

Atoms in this family have 3 valence electrons.This family includes a metalloid (boron), and the rest are metals.This family includes the most abundant metal in the earth's crust (aluminum).



Carbon Family

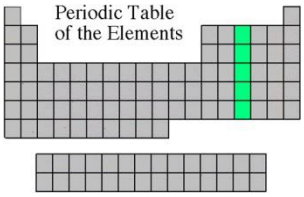
Atoms of this family have 4 valence electrons. This family includes a non-metal (carbon), metalloids, and metals. The element carbon is called the "basis of life." There is an entire branch of chemistry devoted to carbon compounds called organic chemistry. The nitrogen family is named after the element that makes up 78% of our atmosphere.



Inorganic Chemistry

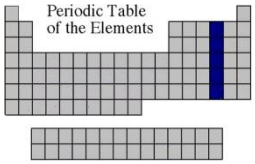
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Nitrogen Family



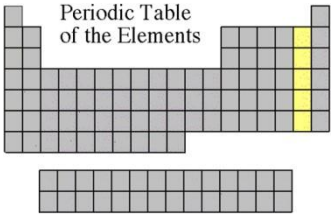
This family includes non-metals, metalloids, and metals. Atoms in the nitrogen family have 5 valence electrons. They tend to share electrons when they bond. Other elements in this family are phosphorus, arsenic, antimony, and bismuth.

Oxygen Family



Atoms of this family have 6 valence electrons. Most elements in this family share electrons when forming compounds. Oxygen is the most abundant element in the earth's crust. It is extremely active and combines with almost all elements.

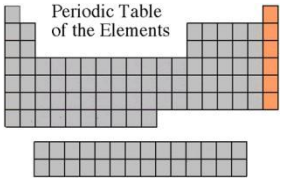
Halogen Family



The elements in this family are fluorine, chlorine, bromine, iodine, and astatine. Halogens have 7 valence electrons, which explains why they are the most active non-metals. They are never found free in nature. Halogen atoms only need to gain 1 electron to fill their outermost energy level. They react with alkali metals to form salts.

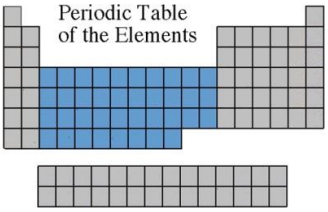
Noble Gases

Noble Gases are colorless gases that are extremely un-reactive.



One important property of the noble gases is their inactivity. They are inactive because their outermost energy level is full. Because they do not readily combine with other elements to form compounds, the noble gases are called inert. The family of noble gases includes helium, neon, argon, krypton, xenon, and radon. All the noble gases are found in small amounts in the earth's atmosphere.

Transition Elements:



Transition Elements include those elements in the B families. These are the metals you are probably most familiar: copper, tin, zinc, iron, nickel, gold, and silver. They are good conductors of heat and electricity. The compounds of transition metals are usually brightly colored and are often used to color paints. Many transition metals combine chemically with oxygen to form compounds called oxides.

Inner Transition Elements

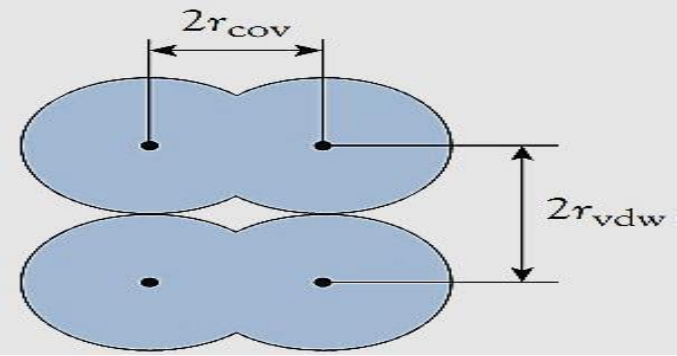
Lanthanoids (the fourteen elements after Lanthanum) and actinides (the fourteen elements after actinium) are called inner transition elements. They are also called f-block elements. The elements after uranium are also called transuranic elements.

Periodic properties

Atomic Radius: There are two common ways in which we can define atomic radius. ***The covalent radius***, r_{cov}, is defined as the half-distance between the nuclei of two atoms of the same element joined in a single covalent bond. The figure below represents the covalent radii (pm) of a typical group and short period.

Be 106	B 88	C 77	N 70	O 66	F 64
					Cl 99
					Br 114
					I 133

The van der Waals radius, r_{vdw}, is defined as the half-distance between the nuclei of two atoms of neighboring molecules. Furthermore, for the metallic elements, it is possible to measure a ***metallic radius***: the half distance between the nuclei of two neighboring atoms in the solid metal. The next figure shows comparison of the covalent radius, r_{cov}, and the van der Waals radius, r_{vdw}.



Covalent radii are experimental values, and there are significant variations in the values derived from different sets of measurements.

* ***In a period, left to right***;
  a- **n** (number of shells) remains constant.
  b- **Z** increases (by one unit).
  c- $\mathbf{Z_{eff}}$ increases (by 0.65 unit).
  d- Electrons are pulled close to the nucleus by the increased $\mathbf{Z_{eff}}$, ***So*** *atomic radius decreases with increase in atomic number (in a period left to right).*

* ***In a group, top to bottom:***
  a- **n** increases.
  b- **Z** increases.
  c- No dramatic increase in $\mathbf{Z_{eff}}$ - almost remains constant. ***So*** *atomic radius increases moving down the group and decreases with increase in atomic number in a period left to right.*

*All anions are larger than their parent atoms, while the cations are smaller.

*The next two tables represent, respectively, the Atomic and Ionic Radii in (pm) unit, where **pm = 10^{-12}m**

Ex: Using only the periodic table rank each set of main-group elements in order of decreasing atomic size: (a) Ca, Mg, Sr (b) K, Ga, Ca

Solution (a) Sr > Ca > Mg. These three elements are in Group 2A (2), and size decreases up the group. (b) K > Ca > Ga. These three elements are in Period 4, and size decreases across a period.

EX: Which of the following atoms has largest radii $_6$C,$_7$N,$_8$O,$_9$F

EX: which of the following has largest radius $_{27}$Co, $_{27}Co^{+2}$, $_{27}Co^{+3}$

Shielding

each electron act as a shell for another electron and reducing the attraction between the nucleus and further electrons. The Z_{eff} increases as a result of the increasing nuclear charge and has a greater and greater effect on the electrons that are being added to orbitals (s and p of the same principal quantum number) that overlap substantially.

Slater's Rules : In 1930, J. C. Slater proposed a set of empirical rules to semiquantify the concept of effective nuclear charge. He proposed a formula that related Z_{eff} to the actual nuclear charge, Z:

$$Z_{eff} = Z - S$$

Where ***s*** is called Slater's screening or shielding constant.Slater derived a series of empirical rules for the calculation of ***s***. The calculation of the screening constant for a specific electron is as follows.

1. The electrons are written in groups as follows:

   1s | 2s 2p | 3s 3p | 3d | 4s 4p | 4d | 4f | 5s 5p | 5d |….

2. All electrons in orbitals of greater principal quantum number ***(at n+1)*** contribute zero.

3. For ***ns*** or ***np*** valence electrons:

   a- Electrons in the same ***ns***, ***np*** group (same principal quantum number) contributes ***(0.35)***.

   b- Electrons in the ***(n-1)*** principal group contribute ***(0.85)***.

   c- Electrons in the ***(n-2)*** or lower groups contribute ***(1.00)***.

4- For ***nd*** and ***nf*** valence electrons:

   a- Electrons in the same ***nd*** and ***nf*** group contribute ***(0.35)***.

   b- Electrons in the groups to the left contribute ***(1.00).***

* For example, to calculate the effective nuclear charge on one of the ***2p*** electrons in the oxygen atom ($1S^2 2S^2 2P^4$), we first find the screening (or shielding constant):

$\boldsymbol{S} = (5 \times 0.35) + (2 \times 0.85) = 3.45$

Hence, $\boldsymbol{Z_{eff} = Z - S} = 8 - 3.45 = 4.55$

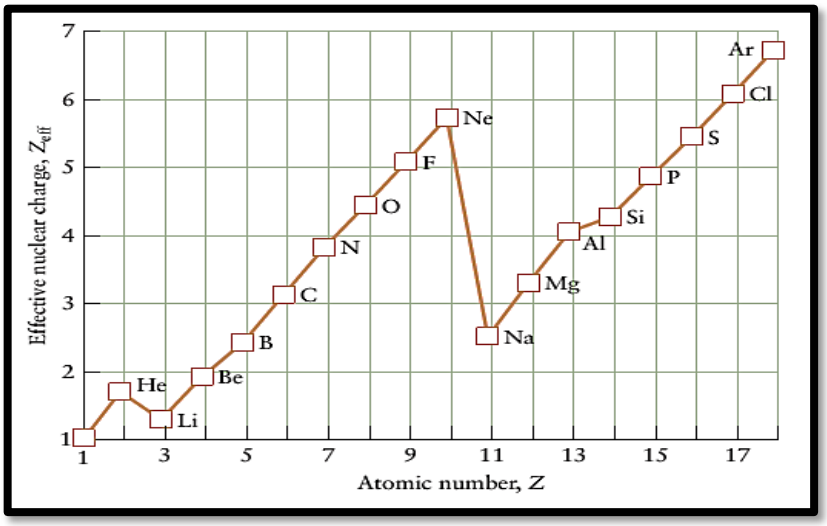
	H							He
Z	1							2
1*s*	1.00							1.69
	Li	**Be**	**B**	**C**	**N**	**O**	**F**	**Ne**
Z	3	4	5	6	7	8	9	10
1*s*	2.69	3.68	4.68	5.67	6.66	7.66	8.65	9.64
2*s*	1.28	1.91	2.58	3.22	3.85	4.49	5.13	5.76
2*p*			2.42	3.14	3.83	4.45	5.10	5.76

Increasing Z_{eff}

As $\boldsymbol{Z_{eff}}$ increases, the orbitals contract, which is why the fluorine atom is smaller than the boron atom. The variation of the effective nuclear charge for the outermost valence electron with atomic number.

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Example: Calculate Z_{eff} **a**-for the last ***3d*** electron of Ni^{28}, **b**-for the 4s electron of Ni^{28}.

Ans. 1- write the electronic configuration of Ni^{28}

$(1s^2)\ (2s^2 2p^6)\ (3s^2\ 3p^6)\ (4s^2)\ (3d^8)$

2- write the Salter's configuration

$(1s^2)\ (2s^2 2p^6)\ (3s^2\ 3p^6)\ (3d^8)(4s^2)$ ×

3- Calculate the shielding constant

$S = [18 \times (1.00)] + [7 \times (0.35)] = 20.45$

$Z_{eff} = Z - S = 28 - 20.45 = 7.55$

For the ***4s*** electron.

$S = [10 \times (1.00)] + [16 \times (0.85) + [1 \times (0.35)] = 23.95$

$Z_{eff} = Z - S = 28 - 23.95 = 4.05$

Other examples**: * Li_3: $1s^2\ 2s^1$** ($Z_{eff} = 3 - [(2\times0.85) + (0\times0.35)] = 1.3$).

* **Na_{11}: $1s^2\ 2s^2\ 2p^6\ 3s^1$ (** $Z_{eff} = 11 - [(2\times1.00)+(8\times0.85) + (0*0.35)] = 2.2$ **).**

Ionization Energy (IE): Is the energy required to remove an electron from a gaseous atom or ion. The losing of an electron is an ***Endothermic*** process (require energy).

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$$M_{(g)} + Energy \rightarrow M^{n+}_{(g)} + e^-$$

Depends on:

a- Size of the atom - IE decreases as the size of the atom increases, thus IE decreases down the group.

b- IE increase from left to right in every period because of the increasing Z_{eff}.

You can calculate ionization energy according to equation below:

$IE = \frac{2\pi^2 m z^{*2} e^4}{n^2 h^2}$, IE= $(Z^{2}*/n^{2})$(IP) when IP=13.6 ev

Ex: calculate the ionization energy of hydrogen atom

$_1H_{(g)} \longrightarrow {}_1H^+(g) + e^-$

$_1H$: $1s^1$ S = 0*0.35= 0 --- Z*= Z-S= 1-0=1

$$IE = \frac{2\pi^2 m z^{*2} e^4}{n^2 h^2} = \frac{2(3.14)^2(9.11 * 10^{-28} g)\ (1)^2(4.8 * 10^{-10} e.s.u)^4}{(1)^2(6.626 * 10^{-27} erq.s)^2}$$

$$= 2.172 * 10^{-11} erq$$

Note:

$$unit = \frac{g.(e.s.u)^4}{erq^2.s^2} = \frac{g.erq^2 cm^2}{erq^2.s^2} = g.cm^2 s^{-2} = erq$$

$$1\ \text{erq} = 6.2419 \times 10^{11} ev$$

$$2.172 * 10^{-11}\ erq\ \frac{6.2419 \times 10^{11} ev}{1 erq} = 13.6\ ev$$

Ex: Calculate the first, second and third ionization energy for Lithium ions ($_3$Li)?

$_3$Li (g)------- Li^{+1} + e

$_3$Li: $1s^2\ 2s^1$

S = 0*0.35+ 2(0.85) = 1.7 Z*= Z-S= 3-1.7= 1.3

$$IE1 = \frac{2\pi^2 m z^{*2} e^4}{n^2\ h^2} = \frac{2(3.14)^2(9.11 * 10^{-28} g)\ (1.3)^2(4.8 * 10^{-10} e.s.u)^4}{(2)^2(6.626 * 10^{-27} erq.s)^2}$$

$$= 9.18 * 10^{-12} erq = 5.73\ ev$$

$_3Li^{+1}$(g) ------ Li^{+2} + e-

$_3Li^{+1}$: $1s^2$

S = 1*0.35= 0.35 ---- Z*= 3- 0.35= 2.65

$$IE2 = \frac{2\pi^2 m z^{*2} e^4}{n^2\ h^2} = \frac{2(3.14)^2(9.11 * 10^{-28} g)\ (2.65)^2(4.8 * 10^{-10} e.s.u)^4}{(1)^2(6.626 * 10^{-27} erq.s)^2}$$

$$= 1.525 * 10^{-10} erq = 95.21\ ev$$

IE_3 = H.W

$_3Li^{+2}$----------Li^{+3} +e –

Li^{+2}: $1s^1$

$^{S=}$ 0*0.35= 0 Z*= Z-S= 3-0= 3

$$IE2 = \frac{2\pi^2 m z^{*2} e^4}{n^2\ h^2} = \frac{2(3.14)^2(9.11 * 10^{-28} g)\ (3)^2(4.8 * 10^{-10} e.s.u)^4}{(1)^2(6.626 * 10^{-27} erq.s)^2}$$

$$= 4.08 * 10^{-14} erq = X\ ev$$

$_2$He: $1s^2$

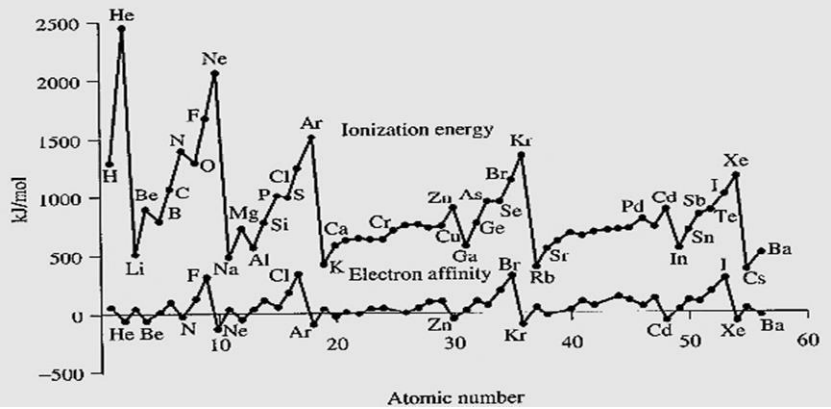
He (g)------ $He^{+1}(g) + e^-$

Electron Affinity (EA)

Electron affinity: is defined as the energy released when an electron is added to an atom. The gaining of an electron is an ***Exothermic*** process (releasing energy).

$$\mathbf{X(g) + e^- \rightarrow X^- (g) + Energy}$$

*The EA of an atom measures the tightness with which it binds an additional electron to itself



On moving across a period, the atomic size decreases and hence the force of attraction exerted by the nucleus on the electrons increases. Consequently, the atom has a greater tendency to attract additional electron i.e., its electron affinity increases.

* EA values of metals are low while those of non-metals are high. Halogens have high electron affinities. This is due to their strong tendency to gain an additional electron to change into the stable ns^2np^6 configuration.

On moving down a group, the atomic size increases and therefore, the effective nuclear attraction decreases and thus electron affinity decreases.

* The next table represents the affinities values of main group elements in KJ/mol

H							**He**
72							−48
Li	**Be**	**B**	**C**	**N**	**O**	**F**	**Ne**
60	≤0	27	122	−8	141 −780	328	−116
Na	**Mg**	**Al**	**Si**	**P**	**S**	**Cl**	**Ar**
53	≤0	43	134	72	200 −492	349	−96
K	**Ca**	**Ga**	**Ge**	**As**	**Se**	**Br**	**Kr**
48	2	29	116	78	195	325	−96
Rb	**Sr**	**In**	**Sn**	**Sb**	**Te**	**I**	**Xe**
47	5	29	116	103	190	295	−77

*__**Electronegativity**__ (EN)

Pauling defined electronegativity as the power of an atom in a molecule to attract shared electrons to itself.

This relative attraction for bonding electron pairs really reflects the comparative $\mathbf{Z_{eff}}$ of the two atoms on the shared electrons. Thus, the values increase from left to right across a period and decrease down a group in the same way as ionization energies do.

Some useful electronegativity values are shown in Figure below:

			H 2.2			
Li 1.0	Be 1.6	B 2.0	C 2.5	N 3.0	O 3.4	F 4.0
			Si 1.9	P 2.2	S 2.6	Cl 3.2
						Br 3.0
						I 2.7

It can calculate electronegativity:

$$EN = \frac{IE + EA}{2}$$

Russell-Saunders Coupling /(TERM SYMBOLE)

• The individual orbital angular momenta of all the electrons combine into a total orbital angular momentum with quantum number L.

• The individual electronic spin angular momenta combine to yield a total spin angular momentum for the whole atom with quantum number S.

• The total atomic angular momentum is given by the coupling of L and S and is described by the quantum number J.

• Atomic or ionic energy levels are characterized by a term symbol of general form: $^{(2S+1)}L_J$

• To obtain a term symbol, the value of L is determined, and assigned the appropriate letter from the series: L 0 1 2 3 4 5 6 7 Symbol S P D F G H I K

$L = \sum m\ell$

L	Symbol
0	S
1	P
2	D
3	F
4	G

• The value of S is used to obtain the spin multiplicity (2S+1) of the term.

• $S = \sum ms$ i.e. the total spin (each unpaired electron = +½).

• Finally the permitted values of J are determined according to the following equation and are known as the levels of the term: $J = \left| L+S \right|, L+S-1, ..., |L-S|$

• The most important term of an atom or ion is the ground term (the most stable term). This can be determined using 3 of Hund's Rules.

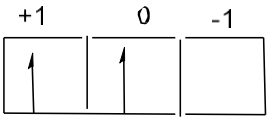
Rule 1: the ground term always has the largest value of S. This is the maximum multiplicity rule.

Rule 2: if two terms have the same multiplicity, the one with the highest value of L lies lowest in energy.

Rule 3: for electronic subshells that are less than half full, the level with the lowest value of J lies lowest in energy. For greater than half-filled subshells, the level with the highest value of J lies lowest in energy.

EX: Determine the possible term symbols and the most stable for each of the following atoms: $_{6}C$, $_{17}Cl$, $_{24}Cr^{+2}$

$_{6}C$: $1s^2\ 2s^2\ 2p^2$



1- $L = \sum m\ell$

$= 1(+1) + 1(0)$

L= 1 ---- P

2- $S = \sum m_s$

$S = (+1/2) + (+1/2)$

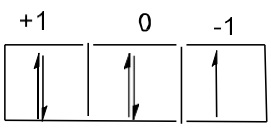
S= 1

3- J= |L+S|, |L+S|-1, |L+S|-2,……|L-S|

2, 1, 0

4- $2S+1 = 2(1) +1 = 3$ $^{2S+1}L_J$

$^{3}P_2$, $^{3}P_1$, $^{3}P_0$ is stable state



$_{17}Cl$: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$

1- L= ∑mℓ

= 2(+1) + 2(0) + 1(-1) = 2-1= 1

L= 1 ----P

2- S= ∑ms

= (+1/2)+(-1/2)+ (+1/2)+(-1/2)+(+1/2)= +1/2

S= +1/2

3- J= $|L+S|, |L+S|-1, |L+S|-2, \ldots\ldots |L-S|$

3/2, 1/2,

2- 2S+1= 2(1/2) +1=2

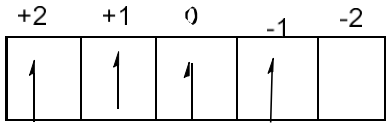
$^2P_{3/2}$, $^2P_{1/2}$

$^2P_{3/2}$ is most stable state

$_{24}Cr: 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^4$

$_{24}Cr: 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1\ 3d^5$

$_{24}Cr^{+2}: 1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^0\ 3d^4$



1- L= ∑mℓ

= 1(+2) + 1(+1) + 1(0)+ 1(-1) = 2+1+0-1= 2

L= 2 ----D

S= ∑ms

= (+1/2)+(+1/2)+ (+1/2)+(+1/2) = 2

S= +2

J= |L+S|, |L+S|-1, |L+S|-2,…… |L-S|

J= 4, 3,2,1,0

4- 2S+1= 2(2) +1=5

$^5D_4$, $^5D_3$, $^5D_2$,$^5D_1$, $^5D_0$

$^5D_0$ is most stable state

H.W: Determine the possible term symbols and the most stable for each of the following atoms: $_{28}Ni$, $_{19}K$, $_{24}Cr$

H.W: find the term symble for stable state of electronic configuration F^5

EX- (X) is a transition element belongs to the **3rd** transition elements series. The ground stable state (term symbol) of its positive ion (X^{3+}) is ($^5D_4$). Predict the atomic number of the element?

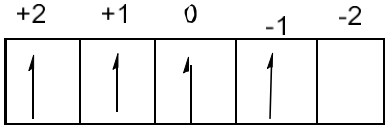
Solution Term symbol is D that means L=2

M= 2S+1= 5 2S= 5-1= 4

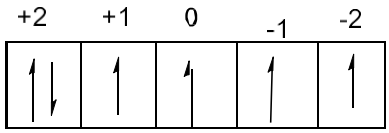
S= 4/2 S= 2

That means there are 4e in 3d and then there are two possible to configuration of the electron

a- The 3d must be less than half filled like



b- The 3d must be more than half



3- Now determine the value of J

J= L+S…..... L-S

(2+2)..... (2-2)

4 …… 0

As the said term symbol is 4 that means the shell must be more than a half filled (possible 2)

4- Write the electron configuration to find atomic number

$X^{+3}= [Xe]_{54}\ 4f^{14}\ 5d^{6}\ 6s^{0}\ 6p^{0} = 74$ 74+3= 77

$X= [Xe]_{54}\ 4f^{14}\ 5d^{7}\ 6s^{2}\ 6p^{0}$

References

1- Inorganic chemistry, F.A Cotton et.al

2- Chemistry of the element, N.N Green wood

3- Atomic Structure & Basic Concepts of Chemistry, Ramesh Duraisam

4- Inorganic chemistry, third addition, Gary L. Miessler &Donald A. Tarr.

5- Inorganic chemistry , fourth addition, James E Huheey; Ellen A. Keiter& Richard L. Keiter

6- Basic inorganic chemistry, third addition, F.Albert Cotton; Goffery Wilkinson& Paul L. Gaus

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