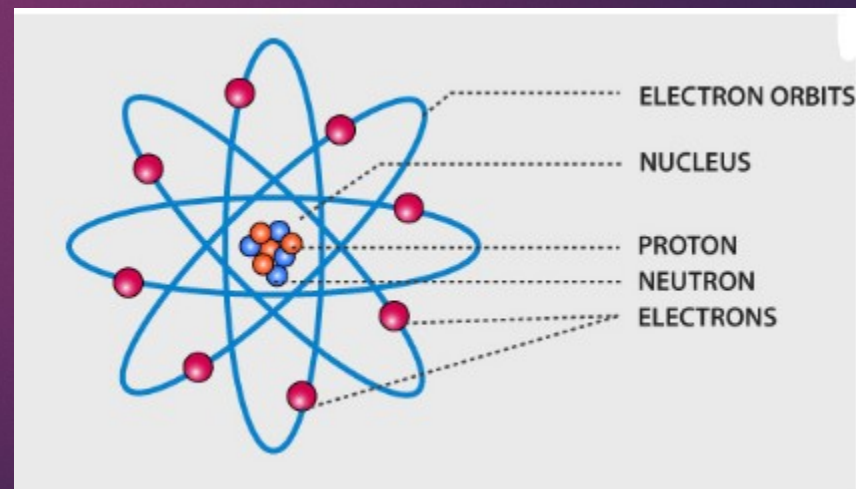


The Atomic Structure

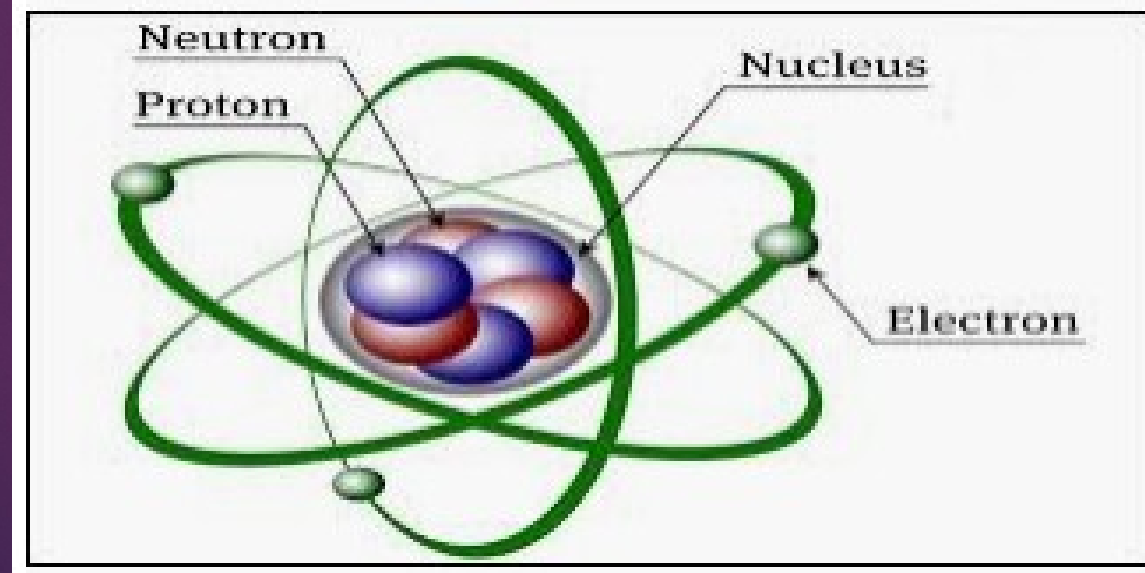


Atomic Structure and Periodicity

Objectives

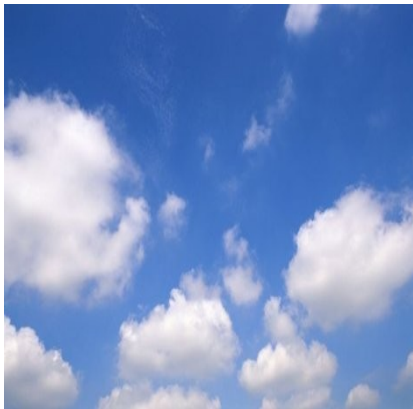
- ▶ What is the evidence of the atom and its structure
- ▶ Describe the properties of electromagnetic radiation.
- ▶ Explain the relationship between energy, frequency, and wavelength.
- ▶ Describe the origin of light emitted by excited atoms and its relationship to atomic structure.
- ▶ Describe the evidence for particle-wave duality.
- ▶ Define the Bohr atomic model and explain how it is flawed.
- ▶ Identify the principles of the quantum mechanical model of the atom.
- ▶ Define the four quantum numbers(n , l , m_l , and m_s) and recognize their relationship to electronic structure.
- ▶ Write the electron configuration for atoms and monatomic ions.
- ▶ How do we explain the trends in the periodic table
- ▶ Explain trends in atom and ion sizes, ionization energy, and chemical properties

Atomic Structure



Atoms

- ▶ Everything is made up of atoms!
- ▶ Here we will try to understand matter (composed of indivisible **tiny units**) in the most basic manner.**An atom!!..**
- ▶ All Matter is Made of Atoms



Dalton's Atomic Theory (1808)

- ❖ John Dalton's theory of the atom started out as a solid sphere with no charges
- ❖ Proposed the atomic theory by investigating atomic weights of atoms
- ❖ formulated a **precise definition** of the indivisible building blocks of matter that we call atoms.



John Dalton (1766–1844)

Hypotheses of Dalton's theory

1. Elements are composed of **extremely small particles**, called **atoms**.
2. All atoms of a given element are identical, having the same size, mass, & chemical properties.
 - ✓ The atoms of one element are different from the atoms of all other elements.

Hypotheses of Dalton's theory

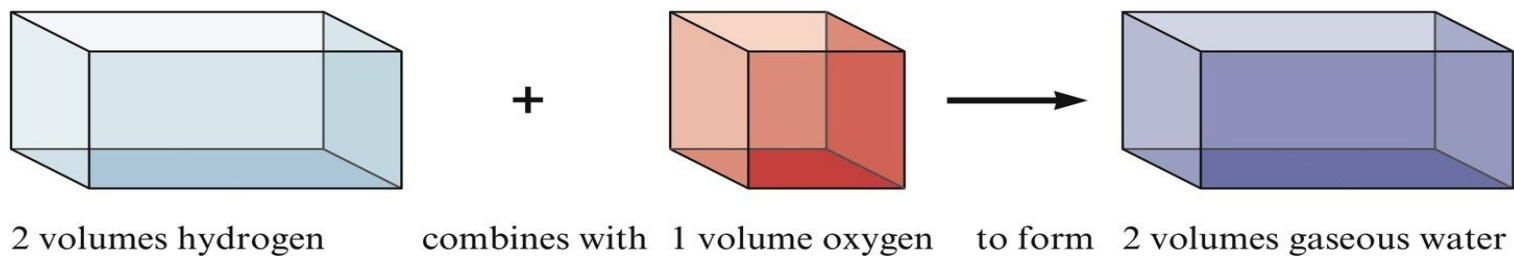
3. Compounds are composed of atoms of more than one element. Chemical compounds are formed when atoms of different elements combine with each other.
 - A given compound always has the same relative numbers and types of atoms.
 - ✓ In any compound, the ratio of the numbers of atoms of any two of the elements present is either an integer or a simple fraction.

Hypotheses of Dalton's theory

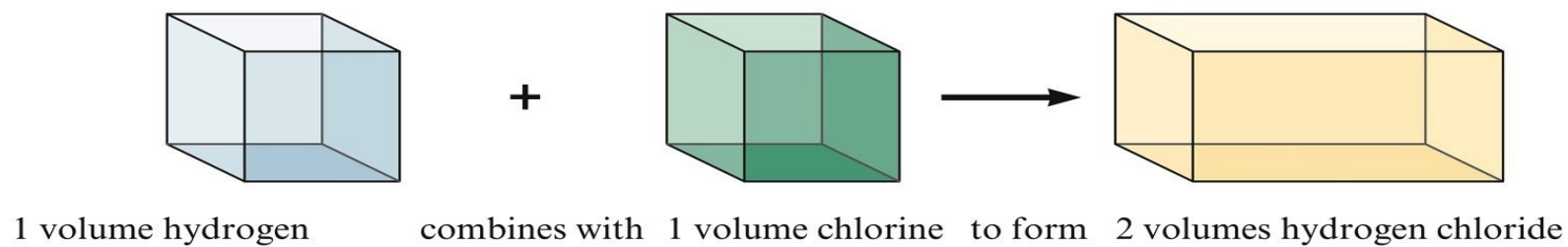
4. A chemical reaction involves only the separation, combination, or rearrangement of atoms; **it does not result in their creation or destruction.**
 - ✓ *Chemical reactions involve reorganization of the atoms—changes in the way they are bound together.*
 - ✓ The atoms themselves are not changed in a chemical reaction.

Representing Gay—Lussac's Results

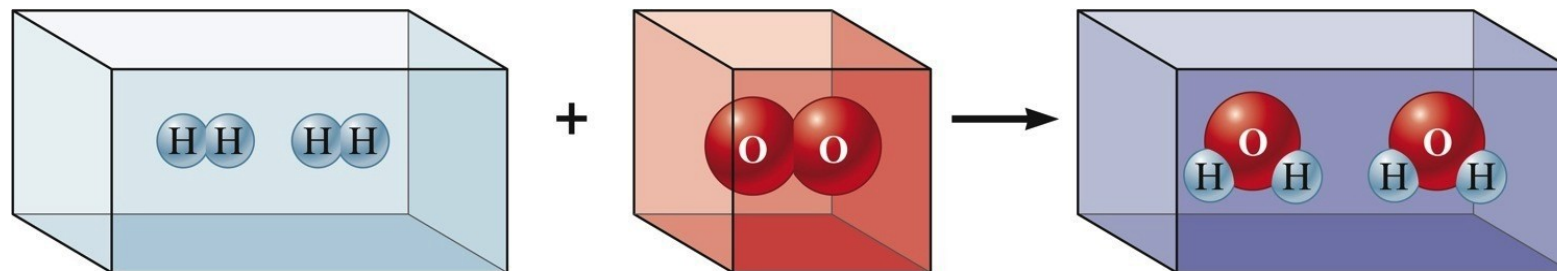
Following the Dalton theory



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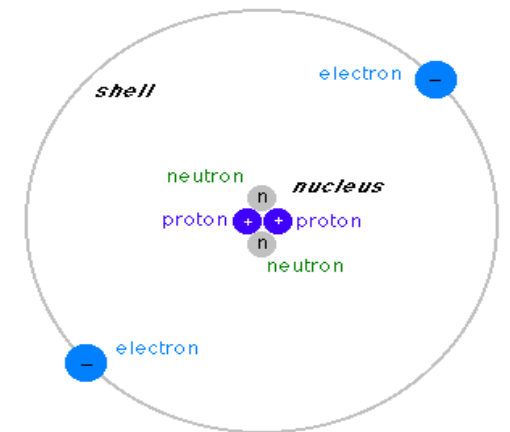
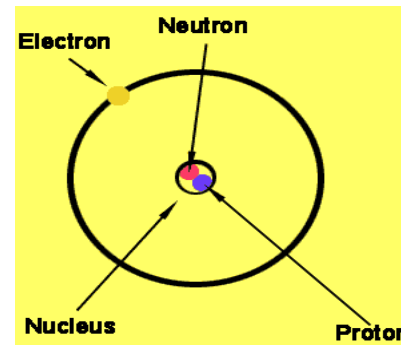


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The Modern view of Atomic Structure

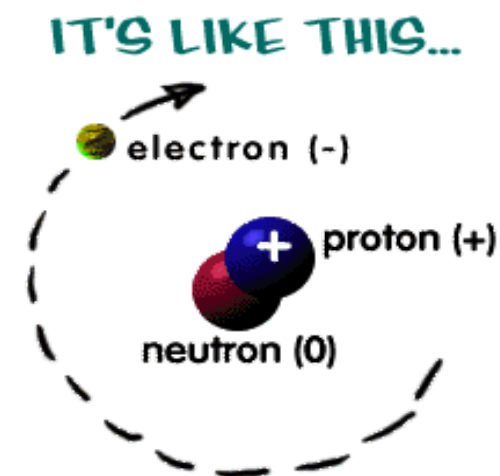
Atoms

- ❖ The smallest particle of an element that has the properties of the element
- ❖ made of 3 basic subatomic particles
- ❖ *there are now many more subatomic particles - theoretical physics*



The atom contains:

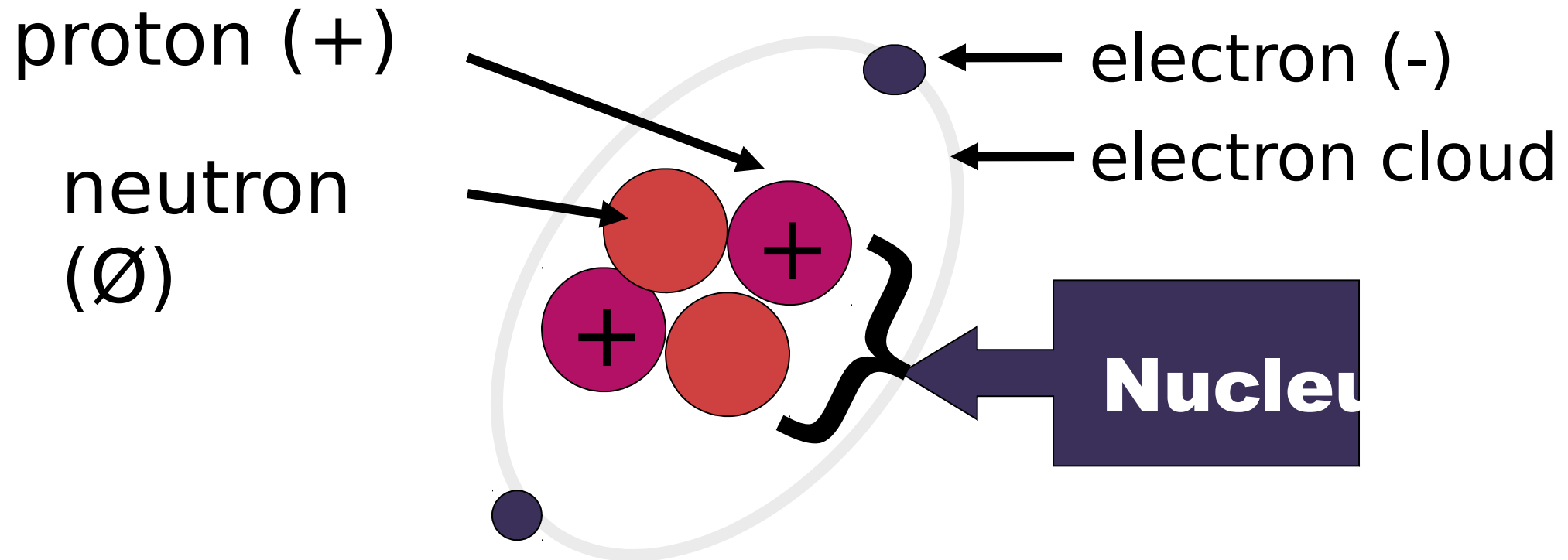
- ▶ **Electrons** – found outside the nucleus; negatively charged.
- ▶ **Protons** – found in the nucleus; positive charge equal in magnitude to the electron's negative charge.
- ▶ **Neutrons** – found in the nucleus; no charge; virtually same mass as a proton.



Subatomic Particles Properties

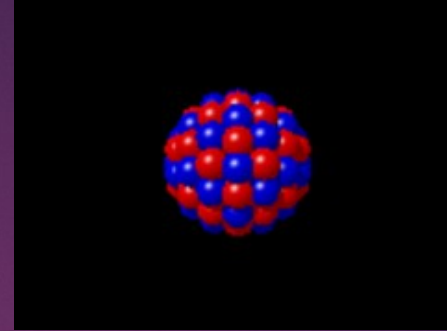
Name	Protons (p or +)	Neutrons (n)	Electrons (e ⁻)
Charge	+1	No charge	-1
Location	in nucleus	in nucleus	in shells around nucleus
Mass	≈ 1 amu	≈ 1 amu	≈ 2000 x smaller
"Job"	Determines identity of element	Supplies proper mass to hold nucleus together	Determines bonding/ how it reacts
Number	Atomic #	Atomic mass - atomic # = # of neutrons	Same as # of protons

Atom Basic Structure

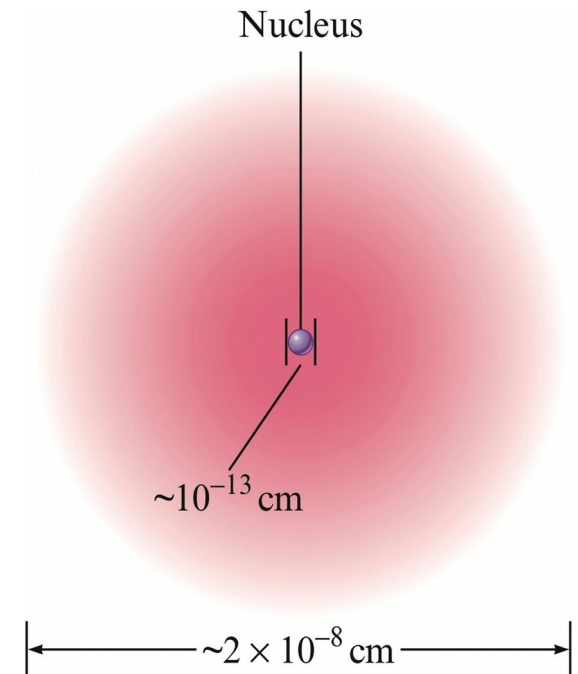


Nucleus: smallest yet heaviest part of the atom

The nucleus:



- ❖ Consist of protons & neutrons
- ❖ Small compared with the overall size of the atom.
- ❖ Extremely dense; accounts for almost all of the atom's mass.
- ❖ Every different atom has a characteristic number of **protons** in the nucleus called the **Atomic Number**.
- ❖ The **mass number** is the total number of protons and neutrons in the nucleus of an atom



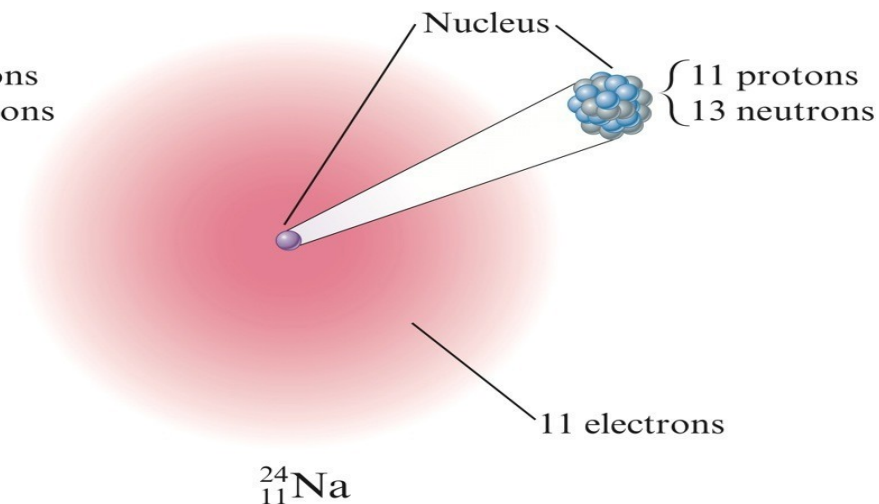
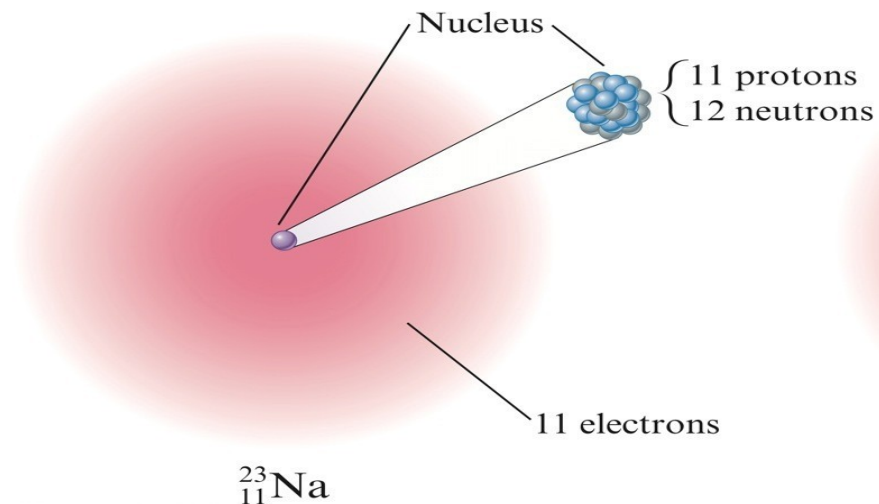
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Nuclear Atom Viewed
in Cross Section

Isotopes

- ❖ Atoms with the same number of protons but different numbers of neutrons.
- ❖ Show almost identical chemical properties; chemistry of atom is due to its electrons.
- ❖ In nature most elements contain mixtures of isotopes.

Two Isotopes of Sodium



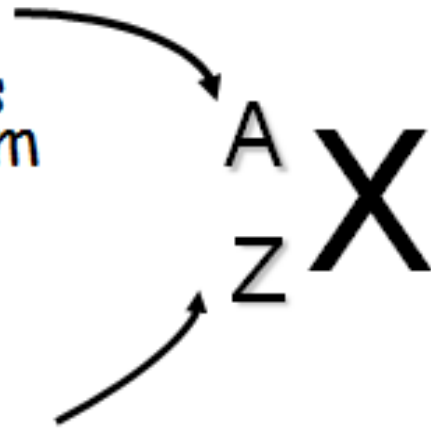
Isotopes are identified by:

Mass number (A)

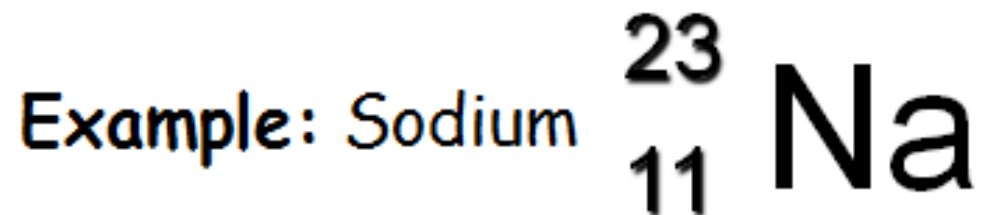
the number of protons and neutrons in an atom

Atomic number (Z)

the number of protons in an atom



Element



EXAMPLE!

A certain isotope X contains 23 protons and 28 neutrons.

- ▶ What is the **mass number** of this isotope?
- ▶ Identify the **element**.

Mass Number = 51

Vanadium

Why atomic structure?

Some questions associated with it

- ❖ World consist of many substances made out of elements, about 100 natural occurring elements.

So...

- ❖ How is that so few elements can lead to such a diverse number of substances?
- ❖ Why does each element have unique physical & chemical properties?

In atomic structure we attempt to answer these questions! !!

Electromagnetic radiation & atomic structure

- ▶ In the 1890s many scientists became caught up in the study of **radiation...**
 - the **emission** & **transmission** of energy (**E**) through space in the form of waves.

- ▶ Information gained from this contributed **greatly** to understanding of **atomic structure**.

Electromagnetic radiation & atomic structure

- ▶ Much information about the electronic structure of atoms comes from observation of the *action of visible light & atoms on each other*.
- ▶ Once it was established that the atom is not indivisible, the scientists made attempts to understand the structure of the atom

Electromagnetic Radiation

Questions to Consider

- ❖ Why Different Colored Fireworks?
- ❖ Why do we get colors?
- ❖ Why do different chemicals give us different colors?



Important points



- ❖ Physical & chemical properties of compounds are influenced by the structure of the atoms that they consist of.
- ❖ Chemical structure depends, in turn, on how electrons are arranged around atoms & how electrons are shared among atoms in molecules.

Important points



23

- ❖ Properties of compounds & atoms rely on a detailed understanding of the arrangement of electrons
- ❖ Arrangement of electrons has been studied by observing how electromagnetic radiation (emr) interacts with atoms.
- ❖ To appreciate the interaction, we ought to understand the nature of emr.!

Electromagnetic radiation

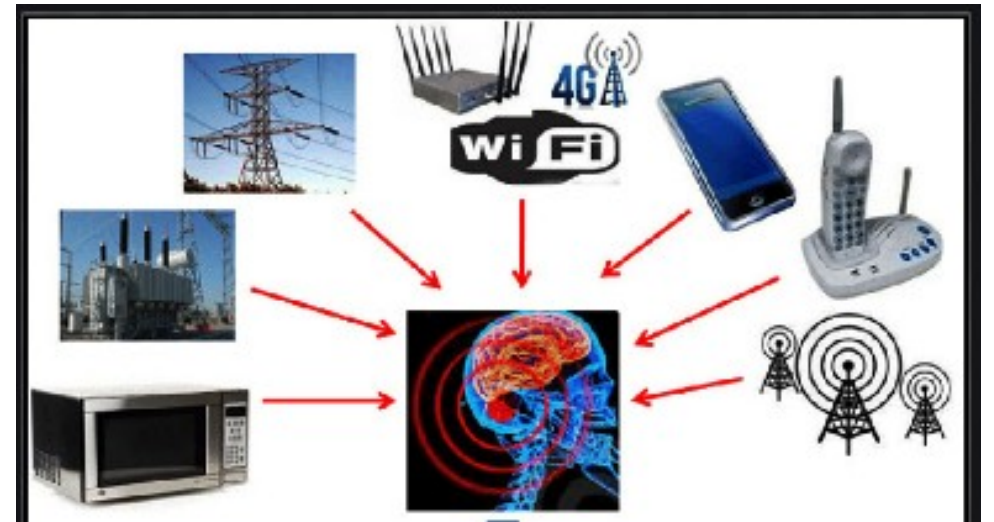
What is EMR?

- ❖ Energy that travels through space as **waves**, is made up of magnetic & electric fields oscillating at **right angles** to one another.
- ❖ type of energy that is commonly known as **light!!**
- ❖ *Light is an electromagnetic wave, consisting of oscillations in electric & magnetic fields traveling through space*

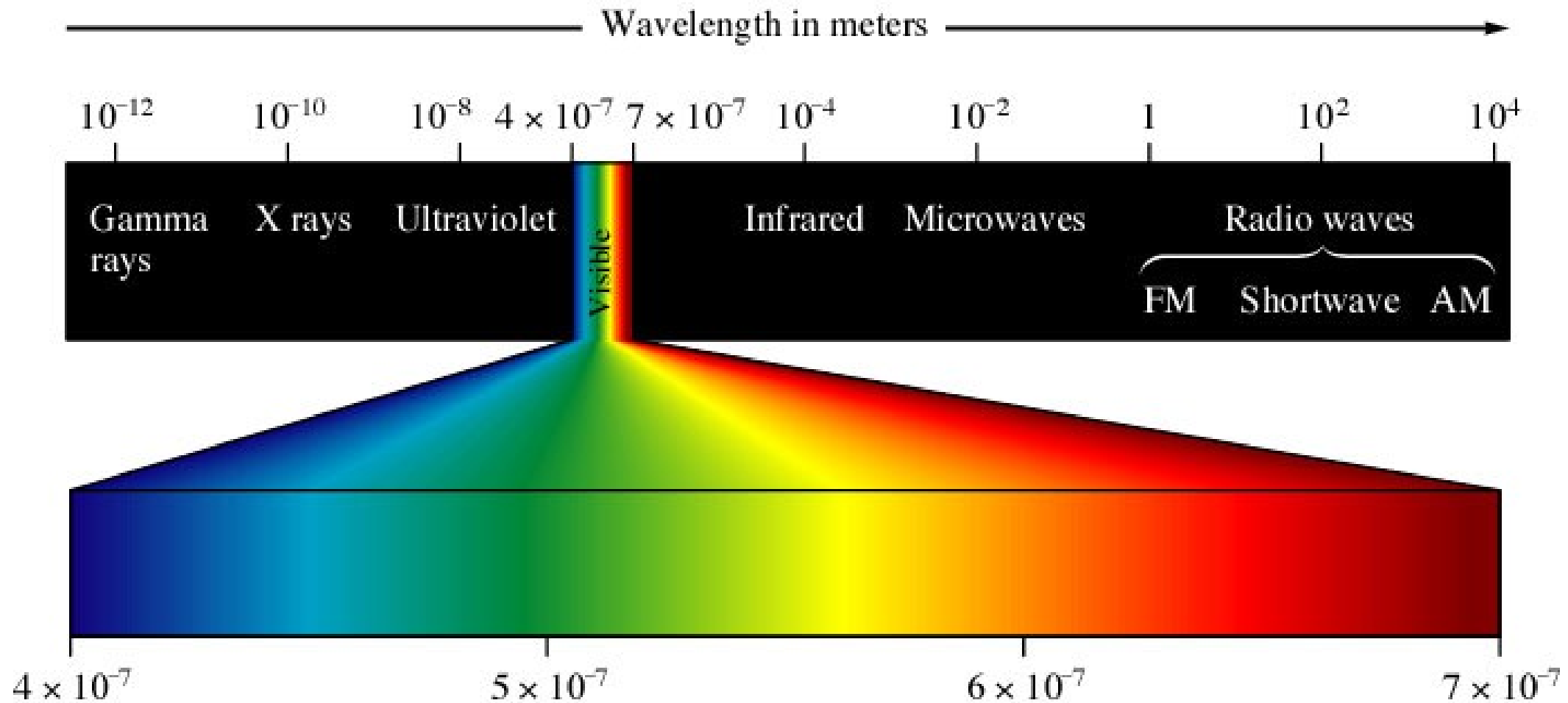
Electromagnetic radiation

EMR is a form of energy that is all around us & takes many forms, such as

- ✓ sunlight,
- ✓ radio waves used by mobile phones,
- ✓ microwaves ovens ,
- ✓ X-rays and gamma rays used in Medicine

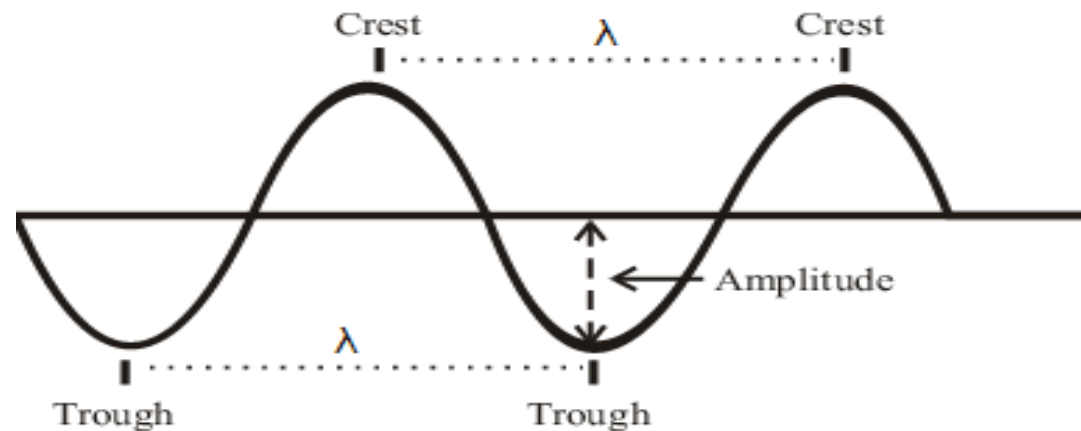


Classification of Electromagnetic Radiation



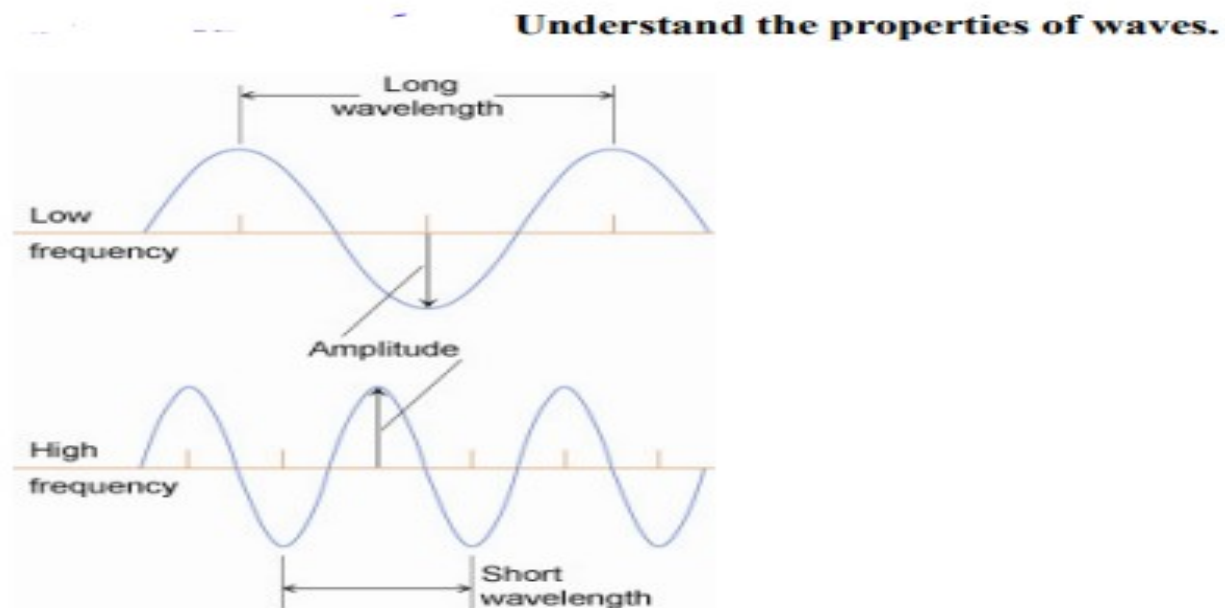
Waves

- ❖ Radiant energy - exhibits wavelike characteristics, travels through space at the speed of light in a vacuum.
- ❖ A wave is a continuously repeating change or oscillation in matter or in a physical field.
- ❖ A wave consists of repeating units called cycles.



Main wave characteristics:

Wavelength (λ) – the distance between two successive crests/peaks (or bottom of two troughs).



Wavelength, frequency, and amplitude

Main wave characteristics:

Frequency (ν, ν) – # of crests or troughs that pass through a given point per unit time.

- ✓ has units of time^{-1} , usually per second (s^{-1}) or Hertz.

$$1\text{Hz}=1/\text{s} \text{ or } 1\text{Hz}=1 \text{ s}^{-1}$$



Amplitude : refers to the maximum height to which the wave oscillates.

- ✓ It equals the height of the crests or depth of the troughs.

Main wave characteristics:

Wave number ($\tilde{\nu}$): # of waves per unit length. It is denoted as $\bar{\nu}$ (ν bar, $\tilde{\nu}$)

It is equal to the reciprocal of the wavelength.

- ✓ The SI unit of $\tilde{\nu}$ is m^{-1} . Sometimes expressed as cm^{-1}

Main wave characteristics:



Velocity: it is defined as the linear distance travelled by the wave in 1 sec.

- ✓ The velocity of a radiation depends on the medium.
- ✓ In a vacuum the velocity is equal to $2.998 \times 10^8 \text{ m s}^{-1}$.

Electromagnetic radiation

have 3 primary characteristics:

1. **Wavelength (λ)**: distance between two consecutive peaks in a wave.
2. **Frequency (ν)** number of waves (cycles) per second that pass a given point in space.
3. **Speed**: speed of light is $2.9979 \times 10^8 \text{ m/s}$. We will use $3.00 \times 10^8 \text{ m/s}$.

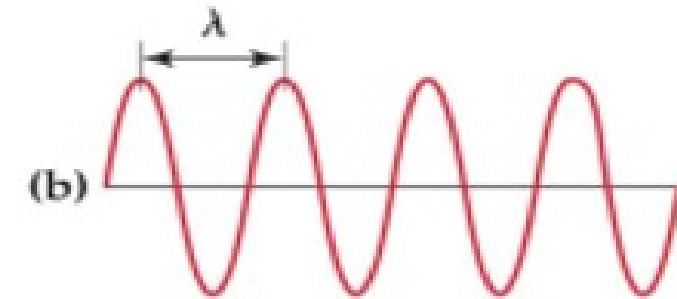
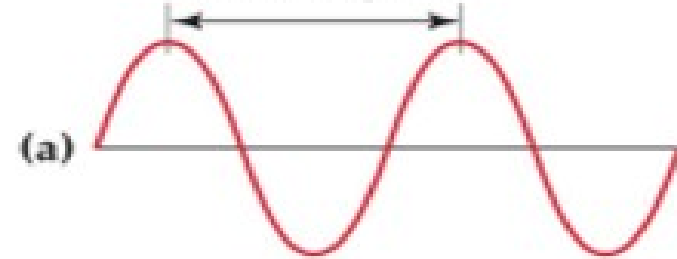


The frequency is the number of complete waves passing any point per second.



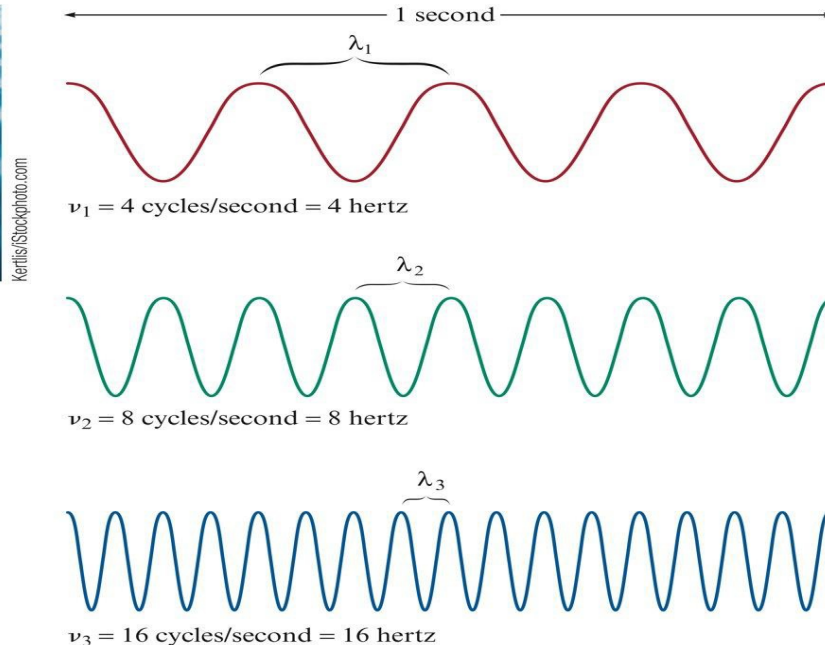
Waves

Wavelength λ



Properties of waves

- ❖ Wave with shortest λ has the highest frequency
- ❖ Wave with longest λ has the lowest frequency,
- ❖ Hence λ is inversely proportional to frequency (ν)



Wavelength & frequency can be interconverted & they have an inverse relationship

$$\nu = c/\lambda$$

ν = frequency (s⁻¹)

λ = wavelength (m)

c = speed of light (m s⁻¹). All types of electromagnetic radiation travel at the same speed, 2.998 X 10⁸ m/s

- ▶ Wavelength is also given in nm (1 nm = 10⁻⁹ m) and Angstroms (Å) (1 Å = 10⁻¹⁰ m).
- ▶ The frequency value of s⁻¹ or 1/s is also called “hertz (Hz)” like KHz on the radio.

EXAMPLE!

When green light is emitted from an oxygen atom it has a wavelength of 558 nm. What is the frequency?

We know,

$$\nu = c/\lambda \quad \text{where, } c = \text{speed of light} \\ = 3.00 \times 10^8 \text{ m/s}$$

$\lambda = \text{wavelength}$

$$= 558 \text{ nm}$$

(need to convert in m)

$$558 \text{ nm} \times \frac{10^{-9} \text{ m}}{1 \text{ nm}} = 5.58 \times 10^{-7} \text{ m}$$

$$\begin{aligned} \nu &= \frac{3.00 \times 10^8 \text{ m} \cdot \text{s}^{-1}}{5.58 \times 10^{-7} \text{ m}} \\ &= 5.38 \times 10^{14} \text{ s}^{-1} \\ &= 5.38 \times 10^{14} \text{ Hz} \end{aligned}$$

The electromagnetic spectrum (range)

- ❖ Gives the classification of the electromagnetic radiations, it is a list of light arranged in order of increasing wavelength
- ❖ In a vacuum, light & other EMR can be identified quantitatively by either **wavelength or frequency.**

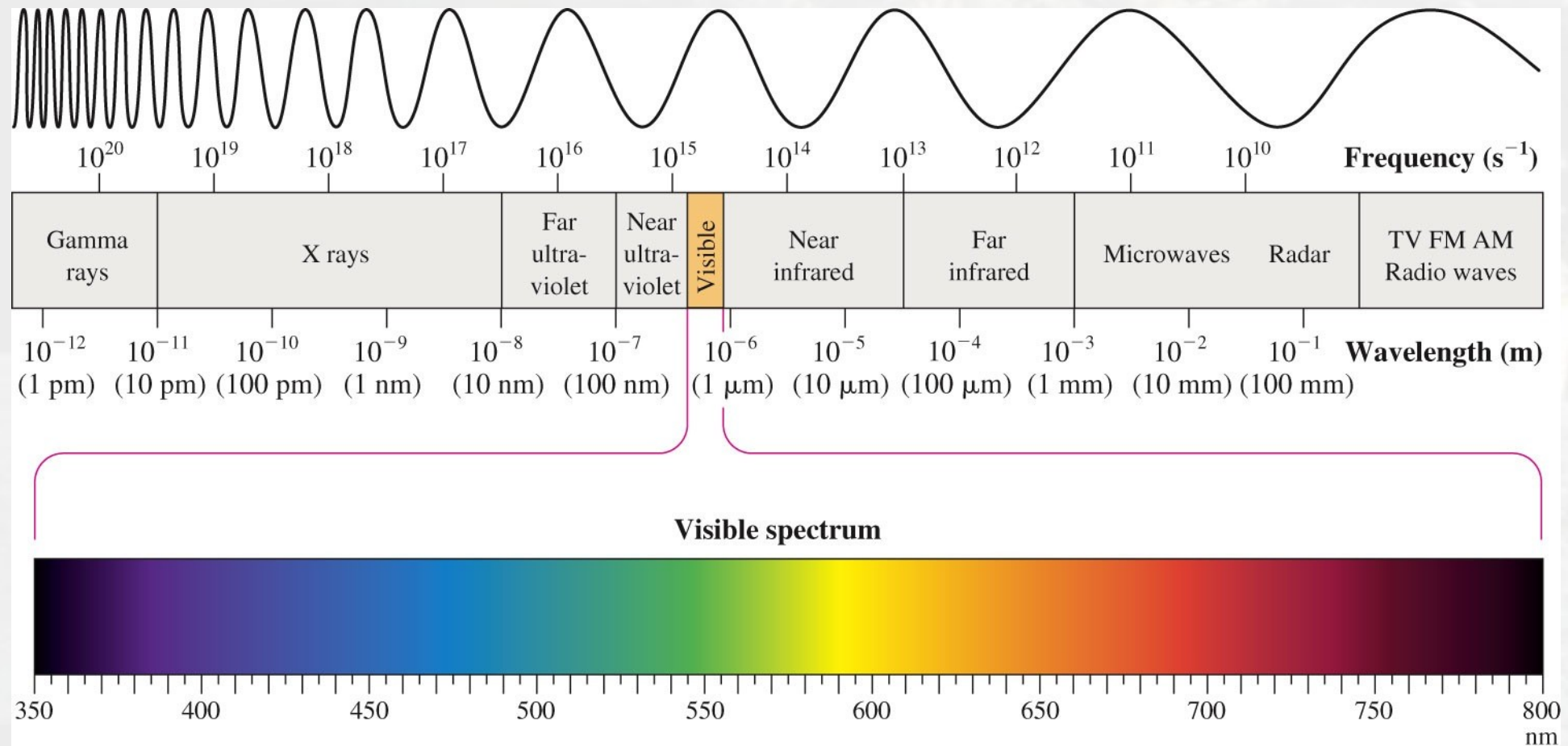
The electromagnetic spectrum (range)

- ❖ **Depending on their characteristics (wavelength , frequency & wave number)....**

... EMR are of many types & constitute what is called as an electromagnetic spectrum.

- ❖ **The part of the spectrum that we can see is called visible spectrum & is a very small part of the** 

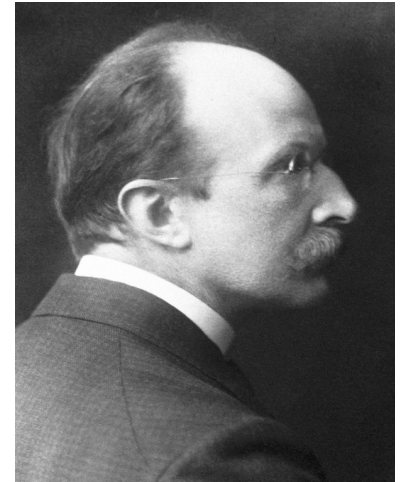
The range of frequencies & wavelengths of electromagnetic radiation is called the **electromagnetic spectrum**.



The Nature of Matter

Max Planck

- ❖ A German physicist, best known as the originator of the quantum theory of energy for which he was awarded the Nobel Prize in 1918.
- ❖ Contributed significantly to the understanding of atomic & subatomic processes.
- ❖ Proposed that energy is radiated in very minute & discrete quantized amounts or packets rather than in a continuous unbroken wave.
 - ▶ postulated that energy can be gained or lost only in *whole-number multiples* of the quantity $nh\nu$, where h is a constant called **Planck's constant**



Max Planck
(1858–1947)

Planck's Constant

- ❖ Transfer of energy is quantized, and can only occur in discrete units, called **quanta**.

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

ΔE = change in energy, in J

h = Planck's constant, 6.626×10^{-34} J s

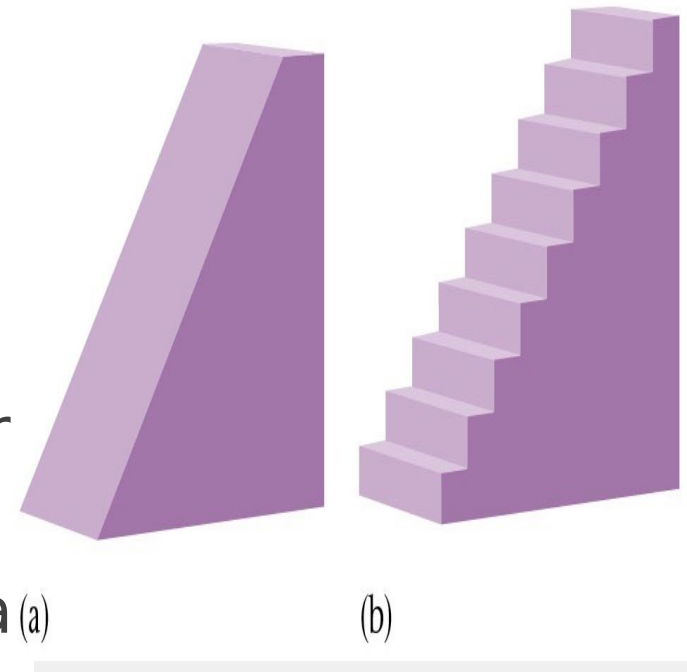
ν = frequency, in s^{-1}

λ = wavelength, in m

- ▶ Electromagnetic radiation is a stream of “particles” called **photons**.

Planck and Quantized Energy

- ❖ Found that energy is quantized.
- ❖ Matter can only absorb or emit certain quantities of energy.
- ❖ Like stairs (b) as opposed to a ramp (a).
- ❖ Energy can be gained or lost only in whole number multiples of $h\nu$.
- ❖ A system can transfer energy only in whole quanta (a) (or packets
- ❖ Energy seems to have particulate properties too.



EMR-The Particulate Nature

- ❖ The energy of the quantum can also be related to the wavelength or wave number as:

$$E = h \frac{c}{\lambda} \text{ or } E = hc\bar{\nu}$$

- ❖ Hence, energy of photon can be readily calculated from these equations if we know the frequency, wavelength or wave number.

EXAMPLE!

The Blue color in fireworks is often achieved by heating copper (I) chloride (CuCl) to about 1200°C. Then the compound emits blue light having a wavelength of 450 nm. What is the increment of energy (the quantum) that is emitted at 4.50×10^2 nm by CuCl?

The quantum of energy can be calculate from the equation

$$\Delta E = h\nu$$

The frequency ν for this case can be calculated as follows:

$$\nu = \frac{c}{\lambda} = \frac{2.9979 \times 10^8 \text{ m / s}}{4.50 \times 10^2 \text{ m}} = 6.66 \times 10^{14} \text{ s}^{-1}$$

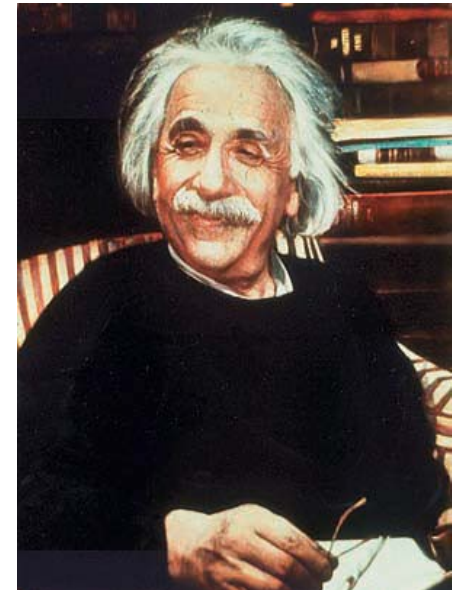
So,

$$\begin{aligned} \Delta E = h\nu &= (6.626 \times 10^{-34} \text{ J}\cdot\text{s})(6.66 \times 10^{14} \text{ s}^{-1}) \\ &= 4.41 \times 10^{-19} \text{ J} \end{aligned}$$

A sample of CuCl emitting light at 450 nm can only lose energy in increments of 4.41×10^{-19} J, the size of the quantum in this case.

The Photoelectric effect

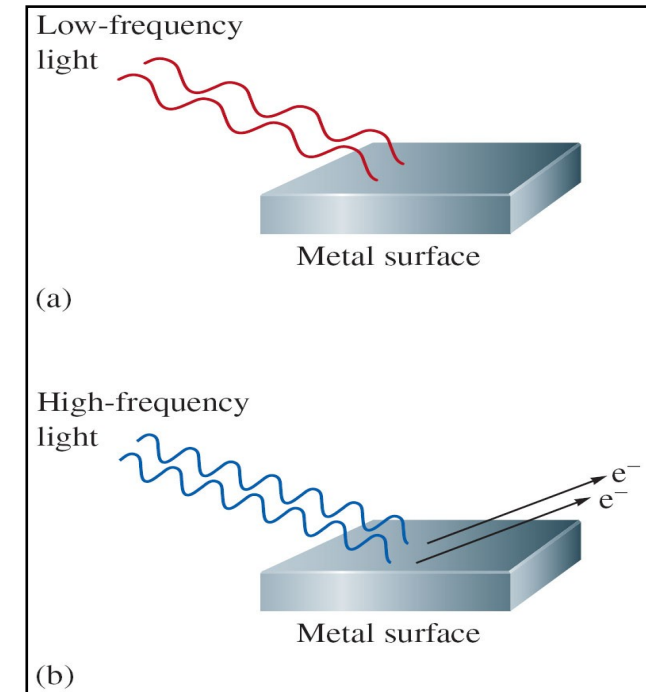
- ❖ In 1887, Heinrich Hertz discovered that certain metals emit electrons when light is incident on them.
- ❖ This was the first instance of light interacting with matter, so it was very mysterious.
- ❖ In 1905 Albert Einstein published a paper which provided the explanation for the effect - light is made up of **small particles**.
- ❖ The **photoelectric effect** is the result of collisions between photons & electrons that knock the electrons out of the metal



Albert Einstein
(1879–1955)

The Photoelectric effect

- ❖ 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**, the electron break free from the atom.
- ❖ Electrons can only leave the surface of the metal if the frequency is above a certain minimum value called the **threshold frequency**
- ❖ Electron emitted are known as **photoelectrons**

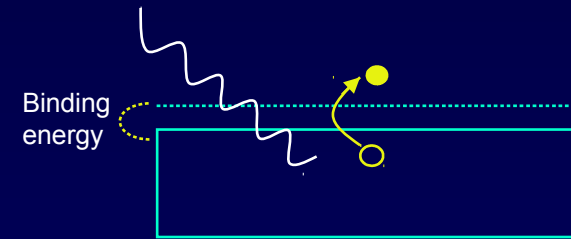


Photoelectric Effect (1)

The energy that bound the electrons to a the metal is called the **work function**, Φ .

If you shine light on a clean metal surface, electrons can emerge if the light gives the electrons enough energy ($> \Phi$) to escape.

Measure the flow of electrons with an ammeter.



Φ is the minimum energy needed to liberate an electron from the metal.

Φ is defined to be positive.

The Photoelectric effect

Photoelectric effect showed that photons transfer all of their energy or none at all

→ Light is made of individual particles (photons)

Electrons are emitted from a metal's surface when struck by light

$$\text{K.E. of electron} = h\nu - h\nu_0 \qquad K.E = \frac{1}{2}m_e v^2 = h\nu - h\nu_0$$

Energy of the photon

Energy required to remove the electron from the metal's surface

If the energy of the photon is less than the threshold $h\nu_0$, electrons are not emitted, no matter how many photons we send. E_0 ($\nu < \nu_0$)

Minimum energy required to remove an electron = $E_0 = h\nu_0$

Energy and Mass

- ❖ According to Einstein theory of relativity-Energy has mass; Einstein equation,

$$E = mc^2$$

where, E = energy, m = mass c = speed of light

- ❖ After rearrangement of the equation,

$$m = \frac{E}{c^2}$$

Now we can calculate the mass associated with a given quantity of energy, **Energy has mass**

Wave-Particle Duality

- ▶ Einstein suggested that electromagnetic radiation can be viewed as a stream of “particles” called **photons**. The energy of each photon is given by,

$$E_{\text{photon}} = h \nu = \frac{h c}{\lambda}$$

$$m_{\text{photon}} = \frac{E}{c^2} = \frac{h c / \lambda}{c^2} = \frac{h}{\lambda c}$$

- ▶ It was then Einstein realized that light could not be explained completely as waves but had to have particle properties. This is called the **dual nature of light**.

Wave-Particle Duality

Dual nature of light:
Electromagnetic radiation (& all matter) exhibits wave properties & particulate properties.



Light as a wave phenomenon



Light as a stream of photons

Electromagnetic Radiation

Photoelectric Effect

Summary of Results:

- Electron energy depends on frequency, not intensity.
- Electrons are not ejected for frequencies below f_0 .
- Electrons have a probability to be emitted immediately.

Conclusions:

- Light arrives in “packets” of energy (photons).
- $E_{\text{photon}} = hf$ ← We will see that this is valid for all objects. It is the fundamental QM connection between an object’s wave and particle properties.
- Increasing the power increases # photons, not the photon energy. Each photon ejects (at most) one electron from the metal.

Recall: For EM waves, frequency and wavelength are related by: $f = c/\lambda$.

Therefore: $E_{\text{photon}} = hc/\lambda$

Beware: This is only valid for EM waves,
as evidenced by the fact that the speed is c .

Summary of the work of Planck & Einstein as follows:

- Energy is quantized. It can occur only in discrete units called quanta.
- EMR, which was previously thought to exhibit only wave properties, seems to show certain characteristics of particulate matter as well. This phenomenon is sometimes referred to as the dual nature of light.
- So, light could under some conditions behave like a particle and other conditions behave as a wave.