Orbitals in Atoms

Electrons they are found in energy levels at different distances away from the nucleus. The positive binding energy is greater for inner shells than for outer shells. The inner shells are closer to the nucleus and so that the electrons feel a greater attractive force. At a certain distance from the nucleus there is a shell with zero energy - this is the boundary of the atom. A large number of unoccupied closely spaced shells exist between the outermost one occupied by electrons and this boundary. Electrons may be raised to these unoccupied shells by a process known as excitation. The exact location of an electron at a given time cannot be pinpointed. However, the most likely location of electrons are represented by atomic orbitals. Atomic orbitals represent where the electrons can be found.

Energy Levels

We picture an atom as a small nucleus surrounded by a much larger volume of space containing the electrons. The lower the number of the principal energy level, the closer the negatively charged electron in it is to the positively charged nucleus and the more difficult it is to remove this electron from the atom. All shells apart from the innermost K-shell consist of more than one sub-shell.

Each principal energy level above the second contains, in addition to one s orbital and three p orbitals, a set of five d orbitals, called the d sublevel. The five d orbitals can hold up to 10 electrons. Thus, the third level holds a maximum of 18 electrons: 2 in the s orbital, 6 in the three p orbitals, and 10 in the five d orbitals.

To distinguish which s, p, d, or f sublevel we are talking about, we precede the letter by the number of the principal energy level. For example, the s sublevel of the second principal energy level is designated 2s; the s sublevel of the third principal energy level is designated 3s; and so on. The number of electrons occupying a particular sublevel is shown by a superscript after the letter of the sublevel.
The energy of an electron versus its orbital

Within a given principal energy level, electrons in p orbitals are always more energetic than those in s orbitals, those in d orbitals are always more energetic than those in p orbitals, and electrons in f orbitals are always more energetic than those in d orbitals. For example, within the fourth principal energy level, we have:

In addition, the energy associated with an orbital increases as the number of the principal energy level of the orbital increases. For instance, the energy associated with a 3p orbital is always higher than that associated with a 2p orbital, and the energy of a 4d orbital is always higher than that associated with a 3d orbital. The same is true of s orbitals:

Describing Atoms

The terms atomic number (Z) and mass number (A) are used to characterize an atom. Atoms whose nuclei have the same atomic number and the same mass number constitute a particular nuclear species or nuclide.
Atomic Number

Neutral atoms of an element contain an equal number of protons and electrons. The number of protons determines an element’s atomic number (Z) and distinguishes one element from another. For example, carbon’s atomic number (Z) is 6 because it has 6 protons. The number of neutrons can vary to produce isotopes, which are atoms of the same element that have different numbers of neutrons.

![Diagram of carbon-12 and helium-4 atoms showing proton and neutron counts]

Mass Number

An element’s mass number (A) is the sum of the number of protons and the number of neutrons. The small contribution of mass from electrons is disregarded in calculating the mass number. This approximation of mass can be used to easily calculate how many neutrons an element has by simply subtracting the number of protons from the mass number. Protons and neutrons both weigh about one atomic mass unit or amu. Isotopes of the same element will have the same atomic number but different mass numbers.

![Diagram of carbon-12 and helium-4 atoms showing mass number]

Isotope

Isotopes are various forms of an element that have the same number of protons but a different number of neutrons. Some elements, such as carbon, potassium, and uranium, have multiple naturally-occurring isotopes. Isotopes are defined first by their element and then by the sum of the protons and neutrons present.

Examples of isotopes are shown << all are isotopes of carbon.
The production of X-Ray

The X-Ray:

X-rays are electromagnetic radiation of exactly the same nature as light but of very much shorter wavelength. Unit of measurement in x-ray region is Å and nm (1 Å = 10^{-10} m, 1 nm = 10 Å = 10^{-9} m)

X-ray wavelengths are in the range 0.5 – 2.5 Å. Wavelength of visible light ~ 6000 Å.

The production of X-Ray:

A high-speed electron can convert some or all of its energy into an X-ray photon when it strikes an atom, and thus we need to speed up electrons to produce X-rays.

The main components of a modern X-ray unit are

(1) a source of electrons—a filament, or cathode;

(2) an evacuated space in which to speed up the electrons;

(3) a high positive potential to accelerate the negative electrons; and (4) a target, or anode, which the electrons strike to produce X-ray.

Steps in the process of X-ray production:

1. The filament of the cathode is heated, causing it to emit electrons.

2. These electrons released from the cathode are repelled by the negative charge of the cathode.

3. A large accelerating potential difference is applied between the cathode and the anode.

4. Then electrons accelerated to high velocity towards the positively charged anode.

5. The electron beam is focused by the use of electric fields onto the anode.

6. These electrons strike the anode and cause it to emit energy as x-ray photons.
With a potential difference in the range 20-150 kV applied between the cathode and the anode, electrons are capable of reaching a very high velocity.

This velocity gives it a relatively large amount of kinetic energy (K.E.) which is given in joules (J) by:

\[ K.E = \frac{1}{2} m v^2 \]

where \( v \) : is the velocity, and \( m \) : An electron's rest mass is \( 9 \times 10^{-31} \) kg.

In an x-ray tube the K.E. of electrons converted to:

- heat (about 99%)
- and x-rays (about 1%) through interactions within the anode.
- So much of the electron energy goes into heating the anode and some into x-ray production by the interact with the innermost (most tightly) bound electrons in the target of anode and "knock" them into excited states.
- When these excited atoms return to their ground state, photons are emitted.
- The maximum energy x-rays correspond to the conversion of the maximum electron beam energy into a photon:

\[ eV = h f_{\text{max}} = h \frac{c}{\lambda_{\text{min}}} \]

where \( V \) : is the accelerating voltage for the tube, \( f_{\text{max}} \) : is maximum x-ray frequency, \( h \) : is Planck's constant, and \( e \): is the electron charge.

**X-ray Interaction With Matter**

When x-rays interact with the body, some are absorbed, some are scattered, and some penetrate to expose the image receptor. So as an x-ray beam passes through a body, three possible fates await each photon:

1. It can penetrate the section of matter without interacting.
2. It can interact with the matter and be completely absorbed by depositing its energy.
3. It can interact and be scattered or deflected from its original direction and deposit part of its energy.

- The number of x-ray photons is **diminished** by passage through body.
- There are two physical processes that are of importance in reducing the number of x-rays:
  1. **Photoelectric effect**: the interaction between the photon and an electron that is **bound** in an atom. In this effect the incident photon gives up its energy to a bound electron in an atom.
  2. **Compton effect** (scattering): the interaction between a photon and a **free** electron. In this interaction the photon looses only a fraction of its energy.

- The number of x-ray photons that emerge decreases as the thickness increases.
- **Photoelectric effect** and **Compton effect** processes determine the absorption coefficient of the material for x-rays:

\[ I = I_0 e^{-\mu \Delta x} \]

where \( I \): is the x-ray intensity at a distance \( x \) in the material, 
\( I_0 \): is the incident intensity of the x-rays. 
\( \mu \): is absorption coefficient of the material, 
\( \Delta x \): is the thickness of the material,

- X-rays are not absorbed equally well by all materials.
- **Heavy** elements such as calcium are much better absorbers of x rays than **light** elements such as carbon, oxygen, and hydrogen. And as a result: structures containing heavy elements (like the bones) stand out clearly.

- The soft tissues (fat, muscles, and tumors) all absorb **equally** well and are thus difficult to distinguish from each other on an x-ray image.

- Air is a poor absorber of x-rays.

- The **lower** energy (soft) x-ray are absorbed more readily than the **higher** energy (hard) x-ray.

- The equivalent energy of an x-ray beam is determined by its half-value layer:

\[
HVL = \frac{0.693}{\mu}
\]

Where \( HVL \): the thickness of a given material that will reduce the beam intensity by one-half (in cm).

\( \mu \) : the linear attenuation coefficient of the attenuating material.

**H.W.** : Find is the HVL for a material with a attenuation coefficient of 0.3/cm

**Properties of x-ray radiation:**

1. X-rays are electrically neutral, that is, they do not experience deviation or deflection when inside an electric, magnetic, or combined field.

2. X-rays travel in straight lines at the speed of light, a characteristic which can be used to direct and focus the rays in order to radiate the specific region of the body being studied.

3. X-rays produce biological and chemical effects, which means they can affect an organism by producing ionization and/or cellular changes that may be responsible for disorders or further mutations.
4. X-rays span a section of the electromagnetic spectrum and possess not only one frequency, but several. These depend on the set of factors that led to the generation of radiation. As shown in figure 1.3, the higher the voltage that produces the rays, the shorter the wavelength is, i.e. the frequency is higher.

5. X-rays are not visible to the human eye or to animals, so their detection is possible only by means of instruments and photographic methods. This is an important consideration in undertaking protective measures for the human body.

6. X-rays produce images on photographic film and fluorescence on certain types of crystals; both phenomena are used as a means to obtain x-rays films and fluoroscopy images on medical monitors, respectively.
The Quantum Theory

Radiation from Incandescent Bodies:

What would you expect to see if you viewed the glowing filament through a diffraction grating? When viewed in this way, all of the colors of the rainbow would be visible. The bulb also emits infrared radiation that you would not see. A plot of the intensity of the light emitted from a hot body over a range of frequencies is known as an emission spectrum, Figure 1.

![Graph showing emission spectra of an incandescent body at three different temperatures.]

Figure 1 This graph shows the emission spectra of an incandescent body at three different temperatures. If you compare the location of each curve’s maximum, you will see that as the temperature increases, the frequency at which the maximum amount of energy is emitted also increases.

The total power emitted by a hot body also increases with temperature. The power (the energy emitted per second) of an electromagnetic wave is proportional to the hot body’s Kelvin temperature raised to the fourth power, $\alpha T^4$. Thus, hotter bodies radiate considerably more power than do cooler bodies.

$$P = \sigma T^4$$

where

- $P$: is the total amount of radiation emitted by an object per square meter (Wattsm$^{-2}$)
- $\sigma$: is a constant called the Stefan-Boltzman constant ($5.67 \times 10^{-8}$ Wattsm$^{-2}K^{-4}$)
- $T$: is the absolute temperature of the object (in K)
The problem with Maxwell’s electromagnetic theory was that it is unable to explain the shape of the spectrum shown in Figure 1. In 1900, German physicist Max Planck assumed that the vibrational energy of the atoms in a solid could have only specific frequencies, as shown by the following equation.

\[ E = nhf \]

**Energy of Vibration**

The energy of a vibrating atom is equal to the product of an integer, Planck’s constant, and the frequency of the vibration.

In the equation, \( f \) is the frequency of vibration of the atom, \( h \) is a constant, called Planck’s constant, with a value of 6.626_10_34 J/Hz, and \( n \) is an integer such as 0, 1, 2, 3 . . .

\[
\begin{align*}
    n = 0: & \quad E = (0)hf = 0 \\
    n = 1: & \quad E = (1)hf = hf \\
    n = 2: & \quad E = (2)hf = 2hf \\

e & \text{and so on}
\end{align*}
\]

Thus, the energy, \( E \), can have the values \( hf, 2hf, 3hf \), and so on, but never values such as \( \frac{2}{3}hf \) or \( \frac{3}{4}hf \). In other words, energy is **quantized**—it exists only in bundles of specific amounts. \( h \) is usually rounded to \( 6.626\times10^{-34}\text{J}\cdot\text{s} \) for calculations.

Planck also proposed that atoms do not always radiate electromagnetic waves when they are vibrating, as predicted by Maxwell. Instead, Planck proposed that atoms emit radiation only when their vibrational energy changes. For example, if the energy of an atom changes from \( 3hf \) to \( 2hf \), the atom emits radiation. The energy radiated is equal to the change in energy of the atom, in this case \( hf \).
The Photoelectric Effect:

Photoelectric effect is the emission of electrons when electromagnetic radiation falls on an object.

The photoelectric effect can be studied in a photocell, such as the one shown in Figure 2. The cell contains two metal electrodes sealed in a tube from which the air has been removed. The evacuated tube keeps the metal surfaces from oxidizing and keeps the electrons from being slowed or stopped by particles in the air. The larger electrode, the cathode, usually is coated with cesium or another alkali metal. The smaller electrode, the anode, is made of a thin wire so that it blocks only a very small amount of radiation. The tube often is made of quartz so as to allow ultraviolet wavelengths to pass through it. A potential difference placed across the electrodes attracts electrons to the anode. When no radiation falls on the cathode, there is no current in the circuit. When radiation falls on the cathode, a current is produced, which is measured by the ammeter, as shown in Figure 27-3. The current is produced because the photoelectric effect causes the ejection of electrons, also called photoelectrons, from the cathode. The flow of electrons is the current in the circuit. The electrons travel to the anode, the positive electrode.

Figure 2: In the photocell shown, electrons ejected from the cathode flow to the anode, completing the circuit and generating an electric current.
Threshold frequency:

Not all radiation falling on the cathode results in a current. Electrons are ejected from the cathode only if the frequency of the radiation is greater than a certain minimum value, called the threshold frequency, $f_0$. The threshold frequency varies widely, depending on the type of metal. No matter how intense, radiation with a frequency below $f_0$ will not cause the ejection of electrons from metal. Conversely, even very low-intensity radiation with a frequency at or above the threshold frequency causes the immediate ejection of electrons. When the incident radiation’s frequency is equal to or greater than the threshold frequency, increasing the intensity of the radiation causes an increase in the flow of photoelectrons.

Photons and quantized energy:

In 1905, Albert Einstein published a theory that explained the photoelectric effect. According to Einstein, light and other forms of electromagnetic radiation consist of discrete, quantized bundles of energy, each of which was later called a photon. The energy of a photon depends on its frequency.

Energy of a Photon $E = hf$

$f$: is frequency in Hz, and $h$ is Planck’s constant in J/Hz. Because the joule is too large a unit of energy to use with atomic-sized systems, the more convenient energy unit of the electron volt (eV) is usually used. One electron volt is the energy of an electron accelerated across a potential difference of 1 V.

$$1eV = 1.60 \times 10^{-19}J$$
H.W:

- Prove the energy of photon is $E = \frac{hc}{\lambda} = \frac{1240 \text{ eV} \cdot \text{nm}}{\lambda}$

- An electron has an energy of 2.3 eV. What is the energy of the electron in joules?

$$ (2.3 \text{ eV}) \left( \frac{1.60 \times 10^{-19} \text{ J}}{1 \text{ eV}} \right) = 3.7 \times 10^{-19} \text{ J} $$

- The threshold wavelength of zinc is 310 nm. Find the threshold frequency, in Hz.

$$ f_0 = \frac{c}{\lambda_0} = \frac{3.00 \times 10^8 \text{ m/s}}{310 \times 10^{-9} \text{ m}} = 9.7 \times 10^{14} \text{ Hz} $$

- Distinguish the photoelectric effect from the Compton effect.
The Compton effect is the scattering of a photon by matter, resulting in a photon of lower energy and momentum. The photoelectric effect is the emission of electrons from a metal sample when radiation of sufficient energy is incident on it.

- What is the energy, in eV, of the photons produced by a laser pointer having a 650-nm wavelength?

$$ E = \frac{hc}{\lambda} = \frac{1240 \text{ eV} \cdot \text{nm}}{650 \text{ nm}} = 1.9 \text{ eV} $$

- An X ray is absorbed in a bone and releases an electron. If the X ray has a wavelength of approximately 0.02 nm, estimate the energy, in eV, of the electron.

$$ E = \frac{hc}{\lambda} = \frac{1240 \text{ eV} \cdot \text{nm}}{0.02 \text{ nm}} = 6 \times 10^4 \text{ eV} $$
The Compton Effect:

The photoelectric effect demonstrates that a photon, even though it has no mass, has kinetic energy just as a particle does. In 1916, Einstein predicted that the photon should have another particle property: momentum. He showed that the momentum of a photon should be equal to \((E/c)\). Because \(E=hf\) and \(\left(\frac{f}{c} = \frac{1}{\lambda}\right)\), the photon’s momentum is given by the following equation.

\[
\text{Photon Momentum} \quad P = \frac{hf}{c} = \frac{h}{\lambda}
\]

The momentum of a photon is equal to Planck’s constant divided by the photon’s wavelength.

Experiments done by an American physicist, Arthur Compton, in 1922 tested Einstein’s theory. The results of Compton’s experiments further supported the particle model of light. Compton directed X rays of a known wavelength at a graphite target, as shown in Figure 3a, and measured the wavelengths of the X rays scattered by the target. He observed that some of the X rays were scattered without change in wavelength, whereas others had a longer wavelength than that of the original radiation. These results are shown in Figure 3b. Note that the peak wavelength for the unscattered X rays corresponds to the wavelength of the original incident X rays, whereas the peak wavelength for the scattered X rays is greater than that of the original incident X rays. Recall that the equation for the energy of a photon, \(E = hf\), also can be written as \(E = h\lambda\). This second equation shows that the energy of a photon is inversely proportional to its wavelength. The increase in wavelength that Compton observed meant that the X-ray photons had lost both energy and momentum. The shift in the energy of scattered photons is called the Compton effect.
In later experiments, Compton observed that electrons were ejected from the graphite block during the experiment. He suggested that the X-ray photons collided with electrons in the graphite target and transferred energy and momentum to them. Compton thought that these photon-electron collisions were similar to the elastic collisions experienced by billiard balls, as shown in Figure 4. He tested this idea by measuring the energy of the ejected electrons. Compton found that the energy and momentum gained by the electrons equaled the energy and momentum lost by the photons. Thus, photons obey the laws of conservation of momentum and energy when they are involved in collisions with other particles.

Figure 4: Much like the collision between two billiard balls (a), when a photon strikes an electron, the energy and momentum gained by the electron equal the energy and momentum lost by the photon (b).
Matter Waves:

The photoelectric effect and Compton scattering showed that a massless electromagnetic wave has momentum and energy, like a particle. If an electromagnetic wave has particle-like properties, could a particle exhibit interference and diffraction, as a wave does? In other words, does a particle have wavelike properties? In 1923, French physicist Louis de Broglie proposed just this, that material particles have wave properties.

De Broglie Waves:

The momentum of an object is equal to its mass times its velocity, \( p = mv \). By analogy with the momentum of a photon, \( P = \frac{h}{\lambda} \), de Broglie proposed that the momentum of a particle is represented by the following equation:

\[
P = mv = \frac{h}{\lambda}
\]

The wavelength in the above relationship represents that of the moving particle and is known as the de Broglie wavelength.

According to de Broglie, particles such as electrons and protons should show wavelike properties. Effects such as diffraction and interference had never been observed for particles, to prove that electrons are diffracted just as light is. Thomson aimed a beam of electrons at a very thin crystal. Atoms in crystals are arrayed in a regular pattern that acts as a diffraction grating. Electrons diffracted from the crystal formed the same patterns that X rays of a similar wavelength formed. Figure 27-9 shows the pattern made by diffracting electrons.
The atom, Elementary particles of the atom

Atomic Structure:

Knowledge of the structure of the atom, the nature of electromagnetic radiation and the production of X-rays is fundamental to the understanding of the physics of medical imaging and radiation protection. In order to understand the radiation physics, radioactivity, and radiation interactions, a simplified model of the atom is all that is needed.

The Rutherford-Bohr Model of the Atom:

What is an atom?

An atom is the building block of matter. A simple model of the atom is that developed by Rutherford and Bohr. The atoms consist of three basic particles: protons, electrons, and neutrons. The nucleus (center) of the atom contains the protons (which have a positive electric charge equal to one electronic charge) and the neutrons (no charge). The outermost regions of the atom are called electron shells (orbits) and contain the electrons (negatively charged). The diameter of the outermost shell defines the size of the atom, which is much larger than the size of the nucleus. Atoms have different properties based on the arrangement and number of their basic particles. Atoms are electrically neutral, so the number of protons equals the number of electrons. The electrons and their configuration in shells, determine the chemical properties of the atom.
The hydrogen atom (H) contains only one proton, one electron, and no neutrons. This can be determined using the atomic number and the mass number of the element (see the concept on atomic numbers and mass numbers).

At the center of the atom is the nucleus, which consists of protons and neutrons. Protons and neutrons can be known collectively as nucleons. Protons and neutrons have approximately the same mass, about $1.67 \times 10^{-24}$ grams. Scientists define this amount of mass as one atomic mass unit (amu). Although similar in mass, protons are positively charged, while neutrons have no charge. Therefore, the number of neutrons in an atom contributes significantly to its mass, but not to its charge.

Electrons are much smaller in mass than protons, weighing only $9.11 \times 10^{-28}$ grams, or about 1/2000 of an atomic mass unit. Therefore, they do not contribute much to an element’s overall atomic mass. When considering atomic mass, it is customary to ignore the mass of any electrons and calculate the atom’s mass based on the number of protons and neutrons alone.
The atom, Elementary particles of the atom

1st Class/ Physics of atom

Dr. Siham Jasim

Electrons

- Electrons surround the nucleus.

- Characteristics of electrons are that they:
  - Have negative charge.
  - Have very small mass.
  - Are arranged in shells (orbits) around the nucleus.

Fig << The Rutherford-Bohr model of the atom

The notion that electrons exist in shells around the nucleus is due to Niels Bohr. He proposed this idea to explain the spectrum of radiation emitted by atoms.
• A short-range force between nucleons keeps the nucleus stable.

• It acts between one proton and another, between one neutron and another, and between a proton and a neutron.

• This force that keeps the nucleus together is known as the strong nuclear force or the strong interaction.

**Stability of the Nucleus**

Figure below shows that a strong force of attraction (negative force) exists for nucleon separation below about $10^{-15}$ m and that this changes to a force of repulsion (positive force) at about $10^{-16}$ m. Therefore the nucleons are kept apart at a distance of about $5 \times 10^{-16}$ m. Quite separate from the strong interaction is the electrostatic force of repulsion (Coulomb force) between the positively charged protons. At separations of $10^{-15}$ m to $10^{-16}$ m, the attractive strong interaction is much greater than the repulsive electrostatic force.

**Fig.** Variation of force between nucleons with distance between them.
Electron Shells (Orbits)

Electrons are arranged in shells (orbits) around the nucleus. The innermost electron shell (closest to the nucleus) is called the K-shell. Moving outwards from the K-shell, successive shells are called the L-shell, M-shell, etc.

![Electron shells in an atom of sodium](image)

**Maximum number of electrons**

- The maximum number of electrons that a shell can hold is $2n^2$ where $n$ is the quantum number of the shell. The shells are numbered outwards from the nucleus i.e. for the K-shell $n = 1$, for the L-shell $n = 2$ etc.:
  - The K-shell holds a maximum of 2 electrons
  - The L-shell holds a maximum of 8 electrons
  - The M-shell holds a maximum of 18 electrons

**Bound Electrons**

The electron shells fill up from the innermost shell (K-shell). This figure shows an atom of aluminium which has a total of 13 electrons; the
K and L shells are full and the three remaining electrons are in the M-shell.

The electrons in the shells are called bound electrons. Electrons in different shells have different energies and, since the electrons are held or bound within the atom, these energies are negative. The outermost shells have the greatest (i.e. least negative) energy. Within each shell, the energies of the sub-shells are very close together. For inner shells the energy differences between sub-shells are much smaller than those between shells.

**Fig ✴️ Energy level diagram for aluminium the dashed line corresponds to a shell at zero energy i.e. the outermost limit of the atom**

**Fig ✴️ Energy level diagram showing sub-shells (labelled s and p) in aluminium**