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Chapter 1

Atoms and Molecules

All bio-organisms including you and me are composed of matter. The **matter** is made of combinations of elements. An **element** is a substance that cannot be separated into simpler substances by chemical means. An atom is the smallest particle of an element that retains its (elements) chemical properties. An **atom** of one element is different in size and mass from the atoms of the other elements. They can be broken down into still smaller particles although they lose their chemical identity in this process. To date, 118 elements have been identified, 94 of them occur naturally on Earth and others have been created by scientists via nuclear processes. The cells of all organisms whether they are derived from plant, animal or microbe contains essentially the same 25 elements almost in almost same proportions. Thus, it can be concluded that out of the 118 known elements, only around 25 are essential for terrestrial life (**Table 1**).

Table 1: The elemental composition of living cell

Element by weight	Symbol	Percentage in body
Oxygen	O	65
Carbon	C	18.5
Hydrogen	H	9.5
Nitrogen	N	3.2
Calcium	Ca	1.5
Phosphorus	P	1.0
Potassium	K	0.4
Sulfur	S	0.3
Sodium	Na	0.2
Chlorine	Cl	0.2
Magnesium	Mg	0.1
Trace elements	B, Cr, Co, F, I, Fe, Mn, Mo, Se, Si, Sn, V, Zn	less than 0.1

Elemental composition of Life forms

Although around 25 types of elements can be found in biomolecules, six elements are the most common. These are called the **CHNOPS elements;** the letters stand for the chemical abbreviations of carbon, hydrogen, nitrogen, oxygen, phosphorus, and sulfur. These six elements contribute almost 98% of the total mass of cells and provide the structural elements of protoplasm. From them, the functional components of cells are formed. Carbohydrates and lipids contain C, H, and O while proteins and nucleic acids contain in addition N and S, and N and P respectively. Na, K, Mg, Ca, and Cl is usually found in ionic forms whose concentrations must remain within narrow limits.

The presence of B, Cr, V, Mn, Fe, Co, Cu, Zn, Si, Sn, and Mo, though in ultra-trace amounts, is essential for the functioning of enzymes. These elements are used as inorganic cofactors in the catalytic function of enzymes. Simply relative abundance in seas, crust and atmosphere of earth does not make any element suitable for life. For example, Aluminum is more abundant than carbon, but it donot performs any essential function to life. Surprising these **CHNOPS elements**, all occur in the first three periods of the Periodic Table (**Table 2**). The unique intrinsic chemical properties of CHNOPS elements make them suitable as building blocks for life. Important features required to function as structural elements are

- Small atomic size
- The flexibility to form 1−, 2−, 3− and 4− electron bonds
- The capability to form multiple bonds.

Table 2: The Structural elements of protoplasm. The common elements in cell have been highlighted.

Period	*Group*							
	I	*II*	*III*	*IV*	*V*	*VI*	*VII*	*VIII*
1	**H**							He
2	Li	Be	B	**C**	**N**	**O**	F	Ne
3	Na	Mg	Al	Si	**P**	**S**	Cl	Ar

Small atoms form the tightest and most stable bonds — a distinct advantage for structural elements. **H, O, N and C are the smallest atoms capable of forming 1-, 2−, 3− and 4− electron bonds respectively.** Utilization of all possible types of electron bonds permits maximum versatility in molecular design. So also does the ability to form multiple bonds, a property confined almost entirely to P, S.

Silicon (Si) is in same group of carbon in the periodic table. Like carbon, it can also form bonds with four other atoms at once, form long chains (polymers), and bind to oxygen. It is the second-most abundant element in the Earth's crust after oxygen. It is these chemical similarities between silicon and carbon that have planted the idea of silicon-based life. However, on earth all known life is based on the element carbon. Advantages of carbon-based life as compare to silicon based are:

a. Greater chemical stability of C—C bonds than the Si—Si bonds.

b. The ability of carbon (silicon cannot), to form multiple bonds; for example, the oxides of carbon are diffusible monomeric gases, whereas the oxides of silicon is a viscous polymer.

c. The stability of C—C bonds, but not of Si—Si bonds, to rupture by nucleophilic reagents (electron-rich elements or compounds) such as O_2, H_2O or NH_3.

Similar factors uniquely qualify P and S for utilization in energy transfer reactions. **Energy transfer is facilitated by bonds susceptible to nucleophilic attack.** P and S resemble Si in that P—O—P or S—O—S bonds, like Si—Si bonds, are susceptible to nucleophilic rupture by virtue of their unoccupied third orbitals. However, unlike Si, P and S form multiple bonds (more versatile), a consequence of their smaller atomic diameters.

Structure of an Atom

Each matter is composed of very small particles called **atoms**. In 1803, Dalton proposed following statements that comprise the atomic theory of matter:

1. Matter consists of indivisible atoms.
2. All the atoms of a given chemical element are identical in mass and in all other properties.
3. Different chemical elements have different kinds of atoms and in particular such atoms have different masses.
4. Atoms are indestructible and retain their identity in chemical reactions.
5. The formation of a compound from its elements occurs through the combination of atoms of unlike elements in small whole number ratio.

Dalton's fourth postulate is clearly related to the **law of conservation of mass**. Every atom of an element has a definite mass. Also in a chemical reaction there is rearrangement of atoms. Therefore after the reaction, mass of the product should remain the same. The fifth postulate is an attempt to explain the **law of definite proportions**. A compound is a type of matter containing the atoms of two or more elements in small whole number ratio. Because the atoms have definite mass, the compound must have the elements in definite proportions by mass. Although, at one time, the atoms were conceived to be the smallest particles, subatomic particles were later recognized in due course of time. The 3 fundamental subatomic particles are: **proton, neutron** and **electron**. Besides these fundamental particles, about 35 other atomic particles are also known to exist. Many of them are, however, extremely unstable and they merely represent a bundle of energy.

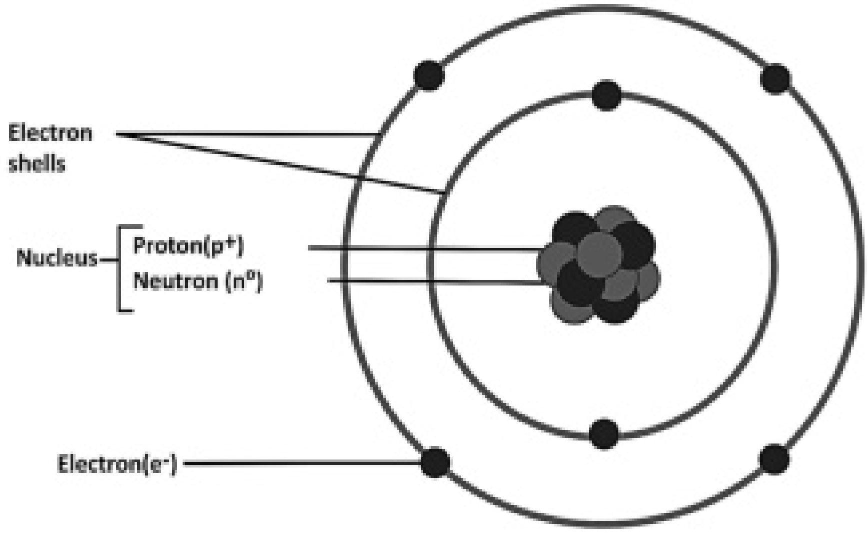

Figure 1: Structure of atom

Regarding the arrangement of fundamental particles inside an atom, **Ernest Rutherford** (1911) proposed the most satisfactory model which is accepted even today with some modifications (**Figure 1**). Each atom has a positively charged nucleus at its center. Nucleus is surrounded by the cloud of negatively charged electrons which are held in a series of orbitals or shells due to electrostatic attraction. The nucleus consists of two kinds of subatomic particles: **protons**, which are positively charged, and **neutrons**, which donot bear charge.

Proton is a subatomic particle, symbol, with a positive electric charge of +1e **elementary charge** and a mass slightly less than that of a neutron. Protons and neutrons, each with masses of approximately one atomic mass unit, are jointly referred to as "**nucleons**"

Neutrons are subatomic particle of about the same mass as a proton but without an electric charge. Neutrons contribute to the structural stability of the nucleus. If there are too many or too few neutrons, the nucleus become unstable and may disintegrate by radioactive decay. Neutrons do not alter the chemical properties of the atom. Thus an atom can exist in several physically distinguishable but chemically identical forms, called isotopes.

Isotopes are atoms of the same element having the same numbers of protons (atomic number), but different numbers of neutrons. They have same chemical properties due to the same electronic configuration but different physical properties. In nature, almost all the elements have multiple isotopes, some of which may be unstable (radioactive).

Radioactivity: The phenomenon of spontaneous emission of certain highly active radiations by radioactive substances is called radioactivity. Three types of radioactive particles are emitted which are alpha (α) rays, beta (β) rays and gamma (γ) rays. The alpha rays have the least penetrating power while the gamma rays have the maximum magnitude.

Alpha rays when pass through electric field show deflection towards negative plate, indicating the presence of positive charge on alpha particles. Each alpha particle has 4 unit mass and two units positive charge therefore alpha particle is same as helium nucleus. An example of a nucleus that undergoes alpha decay is uranium-238. The alpha decay of U-238 is

$$^{238}_{92}U \rightarrow \ ^{234}_{90}U + \ ^{4}_{2}\alpha$$

Beta (negatron) rays get deflected towards positive plate in an electric field and the constituting particles of beta rays are called β particles. Each β particle has mass and charge same as on electron. During beta decay, a neutron splitting into a proton and an electron. The proton stays in the nucleus, increasing the atomic number of the atom by one but mass remain change. The electron is ejected from the nucleus and is the particle of radiation called beta. For example, while most Hydrogen exists as the stable isotope Hydrogen 1, with one proton and no neutrons, heavy isotope Hydrogen 2 (Deuterium) with one proton and one neutron and there are also small amounts of an unstable isotope, the radioactive Hydrogen 3 (Tritium), whose atoms have one proton and two neutrons. Hydrogen 3 undergoes radioactive beta decay at steady rate into stable Helium.

$$^{3}_{1}H \rightarrow \ ^{3}_{2}He + \ ^{0}_{-1}\beta$$

Similarly, most carbon on Earth exists as the stable isotope carbon 12, with six protons and six neutrons, there are also small amounts of an unstable isotope, the radioactive carbon 14, whose atoms have six protons and eight neutrons. Carbon 14 undergoes radioactive beta decay at a slow but steady rate into Nitrogen 14. This forms the basis for a technique known as carbon 14 dating, which is used in archaeology to determine the time of origin of organic materials.

$$^{14}_{6}C \rightarrow \; ^{14}_{7}N + \; ^{0}_{-1}\beta$$

Gamma rays do not show any deflection in electric field and have no charge and carry negligible mass.

$$^{238}_{92}U \rightarrow \; ^{234}_{90}U + \; ^{4}_{2}\alpha + 2^{0}_{0}\gamma$$

In the alpha decay of U-238, two gamma rays of different energies are emitted in addition to the alpha particle.

Isobars are atoms of different elements having **same mass number** but different atomic number. For example carbon (Z=6 , A=12) and nitrogen (Z=7, A=14); another example is potassium (Z=19, A=40) and calcium (Z=20, A=40).

Isotones are the atoms of different elements, which contain **same number of neutrons**. However, both the atomic number and mass numbers are different for the isotones. A few examples include ^{14}C, ^{15}N, ^{16}O are isotones of each other as each has 8 neutrons.

Atomic Number and Atomic mass

Atomic number of any atom is equal to the **number of protons** in the nucleus of an atom and is characteristic of a chemical element and determines its place in the periodic table. An atom of hydrogen has a nucleus composed of a single proton; so hydrogen, with an atomic number of 1, is the lightest element. An atom of carbon has six protons in its nucleus and an atomic number of 6.

The electric charge carried by each proton is exactly equal and opposite to the charge carried by a single electron. Since an atom as a whole is electrically neutral, the number of negatively charged **electrons** surrounding the nucleus is equal to the number of positively charged protons that the nucleus contains; thus the number of electrons in a neutral atom is also equals the atomic number. It is these electrons that determine the chemical behavior of an atom.

Atomic mass: The relative mass of atom or molecule as compare to hydrogen atom is termed as atomic mass or molecular mass respectively. **Atomic mass** is equal to the number of **protons plus neutrons** in atom. **Atomic weight** is the average number of proton and neutron, allowing for the relative abundances of different isotopes. The electrons are ignored because they are much lighter and contribute almost nothing to the total (Almost 1840 times lighter than a proton or neutron). Thus, the major isotope of carbon (^{12}C) has an atomic mass of 12, as it has 6 protons and 6 neutrons whereas the unstable radioactive isotope (^{14}C) has an atomic mass of 14.

	Mass	**Charge**
Proton	1.6726×10^{-27} kg.	1.6022×10^{-19} Coulomb (+ve charge)
Neutron	1.6749×10^{-27} kg.	No charge
Electron	9.1×10^{-31} kg.	1.6022×10^{-19} Coulomb (- ve charge)

Atomic Mass Unit

Dalton or atomic mass units (amu) are standard unit for measuring atomic mass. One Dalton or 1 amu is an atomic mass unit approximately equal to the mass of a hydrogen atom or approximately the mass of one nucleon (either a single proton or neutron) and is numerically equivalent to 1 g/mol. One proton or neutron weighs approximately $1/(6 \times 10^{23})$ gram, so one gram of hydrogen contains 6×10^{23} atoms.

Atoms are so small that it is hard to imagine their size. An individual carbon atom is roughly 0.2 nm in diameter, so that it would take about 5 billion of them, laid out in a straight line, to span a meter. A count of 6×10^{23} atoms or a molecule is called **Avogadro's number**.

It is the key scale factor describing the relationship between everyday quantities and quantities measured in terms of individual atoms or molecules. If a substance has a molecular weight of *X*, then mass of X gram of this substance will have 6×10^{23} molecules. This quantity is called **one mole** of the substance.

One mole has 6×10^{23} atoms or molecules
One mole of carbon weight 12 g
One mole of glucose weight 180 g
One mole of sucrose weight 342 g
One mole of NaCl weight 58 g

Arrangement of Electrons

The electrons are held in a series of **orbitals or shells** of atoms. The electron shells are numbered (from within) as 1, 2, 3, 4, 5, 6 and 7 and are designated by the letters *K, L, M, N, O, P, Q* respectively. Each shell has a certain number of electrons and the maximum number of electrons for each shell is fixed. The maximum number is given by $\mathbf{2n^2}$, where *n* is the serial number of the shell. Thus, the maximum number of electrons in *K, L, M, N, O, P, Q* shells will be 2, 8, 18, 32, 50, 72, 98 respectively. The shells are subdivided into **sub shells.** The number of sub shells in a shell is equal to the number of the shell from within. K shell has one sub shell called *s*; second L shell has two sub shells *s* and *p*; the third M shell has three sub shells *s*, *p* and *d* and fourth N sub shell has four sub shells *s, p, d* and *f*. The sub shells *s, p, d* and *f* can have a maximum of 2, 6, 10 and 14 electrons, respectively (**Table 3**).

Table 3: Distribution of electrons in shells and sub shells

Shell number	1	2		3			4			
Shell name	**K**	**L**		**M**			**N**			
Subshell name	0	0	1	0	1	2	0	1	2	3
Subshell Number	*s*	*s*	*p*	*s*	*p*	*d*	*s*	*p*	*d*	*f*
Number of electron in subshells	2	2	6	2	6	10	2	6	10	14
Total number of electrons in subshell	2	8		18			32			

The electron arrangement of an atom is most stable when all the electrons are in the most tightly bound states that are possible for them—that is, when they occupy the innermost shells. Therefore, with certain exceptions in the larger atoms, the electrons of an atom fill the orbitals in order—the first shell before the second, the second before the third, and so on. An atom whose outermost shell is entirely filled with electrons is especially **stable** and therefore chemically unreactive. Examples are helium with 2 electrons, neon with 2 + 8, and argon with 2 + 8 + 8; these are all inert gases (**Figure 2**).

In contrast, Hydrogen atom has only one electron and thus has a half-filled shell thus is highly reactive. Likewise, the other atoms found in living tissues all have incomplete outer electron shells and are therefore able to donate, accept, or share electrons with each other to form both molecules and ions.

Since atoms with unfilled electron shell are less stable than a filled one, atoms with incomplete outer shells have a strong tendency to interact with other atoms in a way that causes them to either gain or lose enough electrons to achieve a completely filled outermost shell.

This electron exchange can be achieved either by transferring electrons from one atom to another or by sharing electrons between two atoms. Transfer is seen when there is large difference in electro negativities of bonded atom and sharing of electron is seen when there is no difference or very less difference in electronegativities of two bonded atoms. These two strategies generate two types of chemical bonds between atoms: **an ionic bond** is formed when electrons are donated by one atom to another, whereas a **covalent bond** is formed when two atoms share a pair of electrons.

		Electron Shell		
	Electron Shell	I	I	III
1	Hydrogen	●		
2	Helium	● ●		
6	Carbon	● ●	● ● ● ●	
7	Nitrogen	● ●	● ● ● ● ●	
8	Oxygen	● ●	● ● ● ● ● ●	
10	Neon	● ●	● ● ● ● ● ● ● ●	
11	Sodium	● ●	● ● ● ● ● ● ● ●	●
12	Magnesium	● ●	● ● ● ● ● ● ● ●	● ●
15	Phosphorus	● ●	● ● ● ● ● ● ● ●	● ● ● ● ●
17	Chlorine	● ●	● ● ● ● ● ● ● ●	● ● ● ● ● ● ●
18	Argon	● ●	● ● ● ● ● ● ● ●	● ● ● ● ● ● ● ●

Figure 2: Filled and unfilled electron shells in some common elements.

If the pair of electron is shared equally between two bonded atoms, such bonds are termed as **non-polar covalent bonds** but often, the pair of electrons is shared unequally, with a partial transfer between the atoms; this intermediate strategy results in a **polar covalent bond.**

An H atom, which needs only one more electron to fill its shell, generally acquires it by electron sharing, forming one covalent bond with another atom. The other most common elements in living cells—C, N, and O, with an incomplete second shell, and P and S, with an incomplete third shell —generally share electrons and achieve a filled outer shell of eight electrons by forming several covalent bonds. The number of electrons that an atom must acquire or lose (either by sharing or by transfer) to attain a filled outer shell is known as its **valence.**

The crucial role of the outer electron shell in determining the chemical properties of an element means that, when the elements are listed in order of their atomic number, there is a periodic recurrence of elements with similar properties: an element with, say, an incomplete second shell containing one electron will behave in much the same way as an element that has filled its second shell and has an incomplete third shell containing one electron. The metals, for example, have incomplete outer shells with just one or a few electrons, whereas, as we have just seen, the inert gases have full outer shells.

Electronegativity is defined as a measure of the ability of an atom to attract the electron pair in a covalent bond to itself. The value of electronegativity decreases as we go down in any group and increases from left to right in the period. **Oxygen is most electronegative atom in biological system**. The order of electronegativity of some atoms present in biological system is O (3.5) > N (3.0) > S (2.5) =C (2.5) > H (2.1) = P (2.1).

Molecule

A molecule is an aggregate of at least two atoms in a definite arrangement held together by **chemical forces** (also called chemical bonds). It is smallest particle of matter, an element or a compound, which can exist independently. A molecule may contain atoms of the same element or atoms of two or more elements joined in a fixed ratio, in accordance with the law of definite proportions stated. Thus, a molecule is not necessarily a compound, which, by definition, is made up of two or more elements.

Hydrogen gas, for example, is a pure element, but it consists of molecules made up of two H atoms each. Water, on the other hand, is a molecular compound that contains hydrogen and oxygen in a ratio of two H atoms and one O atom. Like atoms, molecules are electrically neutral.

Cells are composed of water, inorganic ions, and carbon-containing (organic) molecules. Among their organic compounds present in organism are **proteins, carbohydrates, nucleic acids** and **lipids** in a significant quantity. The amount of the other types of organic matter is negligible compared to the mass of these four biomolecule groups.