Unit 1

Molecules & their interaction relevant to biology

Unit Map

1.A Structure of atoms, molecules and chemical bonds

1.A.1 Structure of atom

Matter has mass and it occupies space. Atoms are basic building blocks of matter and they are composed of three types of particles such as protons, neutrons and electrons. Protons and neutrons are responsible for most of the atomic mass and are present in the nucleus. Protons have a positive (+) charge, neutrons have no charge i.e. they are neutral. The electrons reside on orbitals around the nucleus. These electrons carry a negative charge (-). The number of protons in an atom determines its atomic number (Z) (e.g. H = 1). The number of protons in an element is constant (e.g. H = 1, U r= 92) but the neutron number may vary, so the mass number (A = protons + neutrons) may vary accordingly. The same element may contain varying numbers of neutrons and have the same number of protons in each atom; these forms of an element are called ***isotopes***. The chemical properties of the isotopes are same, although the physical properties of some isotopes may be different. Some isotopes are radioactive in nature, which means that they radiate energy as they decay to a more stable form, perhaps to another element half-life ($t_{1/2}$); that is the time required for half of the atoms of an element to decay into stable form.

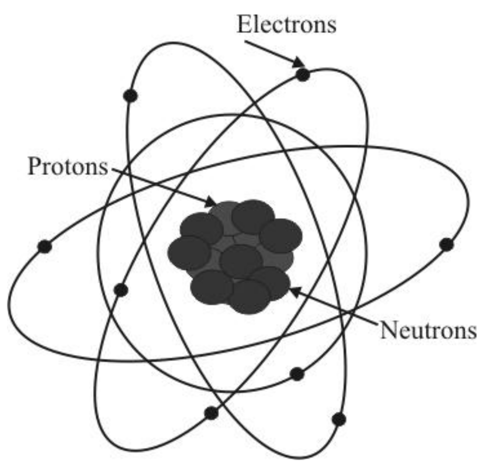


Figure 1.A.1-1
- Atom = protons + neutrons + electrons
- Protons (positively charged) + neutrons (no charge) = atomic mass or mass number (A). (A = Z+N)
- Protons (negatively charged) = atomic number (Z)
- Isotopes = variants of same elements having different no. of neutrons.
- Uncharged atom, atomic number = electrons

Example Carbon and Uranium have three isotopes and written as ^{12}C, ^{13}C, ^{14}C, ^{234}U, ^{235}U, ^{238}U

Example of isotope

The carbon atoms exist naturally with 6, 7 or 8 neutrons. Since each atom of carbon has 6 protons, the isotopes must have atomic masses of 12, 13 and 14. (Since atomic mass = protons + neutrons). These isotopes are called carbon-12, carbon-13 and carbon-14 and they are written as ^{12}C, ^{13}C and ^{14}C. Carbon-12 and carbon-13 are the stable forms of carbon. Carbon-14 is unstable, decaying with a half-life of about 5,700 years. It is produced in earth's atmosphere by cosmic ray bombardment of nitrogen-14. Uranium has three naturally occurring isotopes. These are uranium-234, uranium-235 and uranium-238. Since each atom of uranium has 92 protons, the isotopes must have 142, 143 and 146 neutrons respectively.

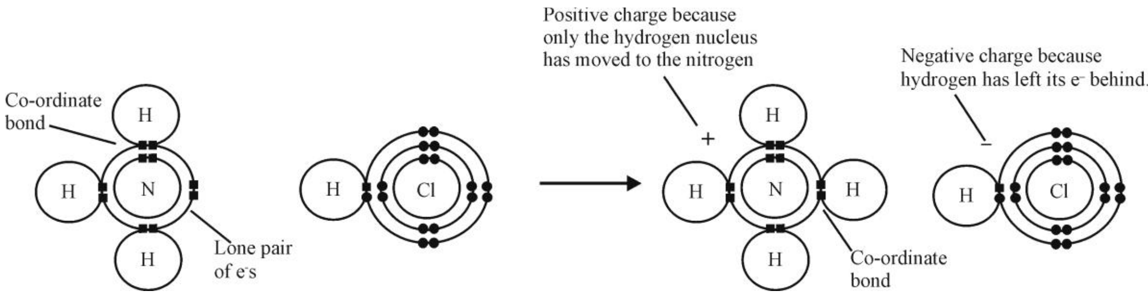
1.A.2 Structure of molecules and chemical bond

Bonds hold atoms and molecules of substances together. There are several different kinds of bonds, which depend on the chemical properties, as well as the attractive forces of the atoms and molecules. The three types of chemical bonds are ***Ionic bonds***, ***Covalent bonds***, ***Co-ordinate bonds (dative covalent bonds), Polar bonds and Hydrogen bonds***

- **Covalent bonds**

  Covalent bond is the bond in which one or more pairs of electrons are shared by two atoms. Covalent bonds are formed when two atoms have a very small (nearly insignificant) difference in their electronegativity. The value of difference in electronegativity between two atoms in a covalent bond is less than 1.7. Covalent bonds are often formed between similar atoms, non-metal to non-metal or metal to metal. The covalent bonding present between, signals a sharing of electrons. Covalent bonds are usually strong in nature.

Examples



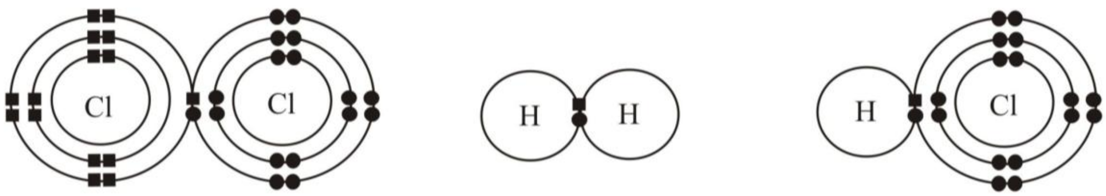


Figure 1.A.1-2
Chlorine Two chlorine atoms could both achieve stable structures by sharing their single unpaired electron. The two chlorine atoms are said to be joined by a covalent bond. The reason that the two chlorine atoms stick together is that the shared pair of electrons is attracted to the nucleus of both chlorine atoms.
Hydrogen atoms only need two electrons in their outer level to reach the noble gas structure of helium. Once again, the covalent bond holds the two atoms together because the pair of electrons is attracted to both nuclei.
Hydrogen Chloride The hydrogen has a helium structure and the chlorine an argon structure.

- **Co-ordinate bond**

  A covalent bond is formed by two atoms sharing a pair of electron. The atoms are held together because the electron pair is attracted by both of the nuclei. In the formation of a simple covalent bond, each atom supplies one electron to the bond-but that does not have to be the case. A co-ordinate bond (also called a dative covalent bond) is a covalent bond (a shared pair of electrons) in which both electrons come from the same atom.

  Example If the colourless gases are allowed to mix, a thick white smoke of solid ammonium chloride is formed.

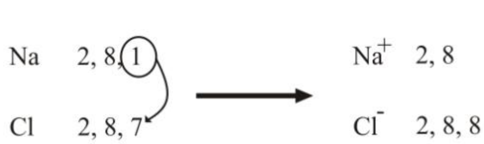
  $NH_3 + HCl \rightarrow NH_4Cl$

  Ammonium ions, NH_4^+, are formed by the transfer of a hydrogen ion from the HCl to the lone pair of electrons on the ammonia molecule.

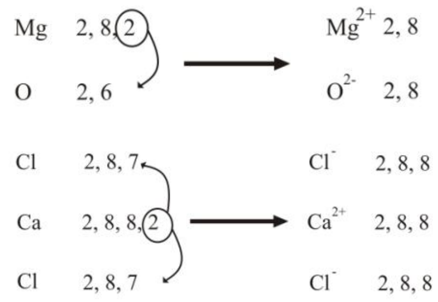
- **Ionic bond**

  The bond in which one or more electrons from one atom is removed and attached to another atom, resulting in positive and negative ions which attract each other. Ionic bonds form when two atoms have a large difference in electronegativity (electronegativity is the quantitative representation of an atom's ability to attract an electron pair of the bond to itself). Ionic bonds often occur between metals and non-metals. Compounds displaying ionic bonds form ionic crystals in which ions of positive and negative charges are near each other. Ionic bonds can typically be broken through hydration-the addition of water to a compound. It is also known as ***electrostatic bond.***

  Examples



- **Sodium chloride** Sodium (2, 8, 1) has 1 electron more than a stable noble gas structure (2, 8). If it gave away that electron it would become more stable. Chlorine (2, 8, 7) has 1 electron short than a stable noble gas structure (2, 8, 8). If it could gain an electron from somewhere it too would become more stable. If a sodium atom gives an electron to a chlorine atom, both become more stable.



- **Magnesium oxide** Similarly Mg and O can attain stable structure by transfer of 2e$^-$ from Mg to O. Again, noble gas structures are formed, and the magnesium oxide is held together by very strong attractions between the ions. The ionic bonding is stronger than in sodium chloride because this time you have 2$^+$ ions attracting 2$^-$ ions. The greater the charge, the greater is the attraction. The formula of magnesium oxide is MgO.
- **Calcium chloride** Two chlorines are required by two outer electrons in the calcium. The formula of calcium chloride is therefore $CaCl_2$.

➢ **Polar bond**

Polar covalent bonds fall between ionic and covalent bonds. They are formed when two elements bond with a moderate difference in electronegativity moderately to greatly. Although polar covalent bonds are classified as covalent, they do have significant ionic properties. They also induce dipole-dipole interactions, where one atom becomes slightly negative and the other atom becomes slightly positive. Polar covalent bonds indicate polar molecules, which are likely to bond with other polar molecules but are unlikely to bond with non-polar molecules.

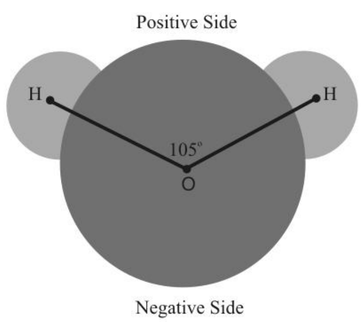


Figure 1.A.2-1
Structure of polar bond
- Polar bond is formed between two elements having different electronegativity.
- Due to this one element gets slightly positive charge and another gets slightly negative charge. i.e. in water molecule, hydrogen gets slightly positive and oxygen gets slightly negative.

➢ **Hydrogen bonds**

A hydrogen bond is a chemical bond in which a hydrogen atom of one molecule is attracted to an electronegative atom, especially nitrogen, oxygen or fluorine atom of another molecule. Hydrogen bonds are very specific and lead to certain molecules having special properties due to these types of bonds. Hydrogen bonding may result in the element that is not hydrogen, for example oxygen having a lone pair of electrons on the atom thus making it polar.

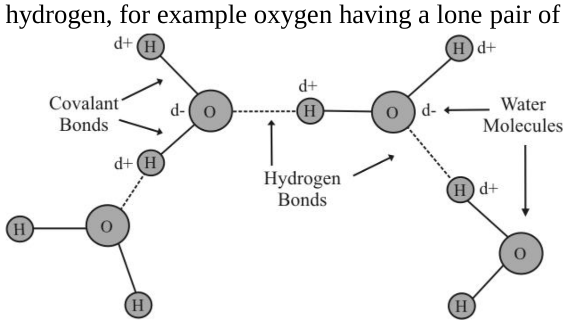


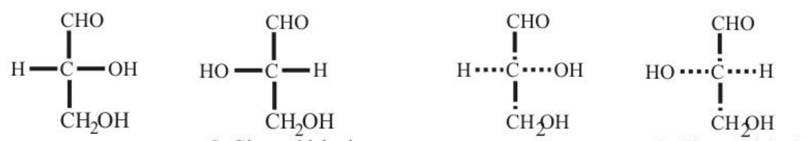
Figure 1.A.2-2
Structure of hydrogen bond in water
- Bond is formed between hydrogen atom and electronegative atom.
- In this figure hydrogen bond is formed between hydrogen atom of one molecule of water and oxygen atom of another molecule.
- Hydrogen bond is shown with dotted line.

1.B Composition, structure and function of biomolecules

1.B.1 Carbohydrates

Carbohydrates are polyhydroxy aldehydes or ketones and their derivatives. The word carbohydrate includes polymers and other compounds synthesized from polyhydroxy aldehydes and ketones. If aldehyde group is present they are called ***aldoses*** if ketones are present they are called ***ketoses***. Chemically, carbohydrates are so named as majority of the molecules are composed of carbon, hydrogen and oxygen in the same ratio as that found in water (H_2O). Simple carbohydrates or the entire carbohydrate family may also be called ***saccharides*** as their main component is sugar. In general carbohydrates have the empirical formula (CH_2O). Carbohydrates may be classified as ***monosaccharides***, ***oligosaccharides*** and ***polysaccharides***.

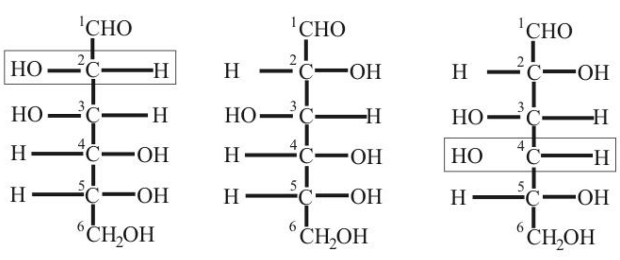
- **Monosaccharide (General formula $C_m(H_2O)_n$)** the carbohydrates, which contain 3-7 carbon atoms, are called ***monosaccharide.*** They are the simplest and smallest unit from which disaccharides, oligosaccharides and polysaccharides are formed. Monosaccharides are either aldehydes or ketones, with one or more hydroxyl groups; the six-carbon monosaccharides glucose (an aldohexose) and fructose (a ketohexose) have five hydroxyl groups. The carbon atoms, to which hydroxyl groups are attached, are often chiral centers and stereoisomerism is common among monosaccharides.
  - On the basis of number of carbon atoms, monosaccharides with three, four, five, six and seven carbon atoms are called trioses, tetroses, pentoses, hexoses and heptoses respectively. Because these molecules have multiple asymmetric carbons, they exist as diastereoisomers, isomers that are not mirror images of each other, as well as enantiomers. In regard to these monosaccharides, the symbols D and L designate the absolute configuration of the asymmetric carbon farthest from the aldehyde or keto group. D-Ribose, the carbohydrate component of RNA, is a five-carbon aldose. D-Glucose, D-mannose and D-galactose are abundant six-carbon aldoses.
  - All the monosaccharides except dihydroxyacetone contain one or more asymmetric (chiral) carbon atoms and thus occur in optically active isomeric forms. The simplest aldose, glyceraldehyde contains one chiral center and therefore has two different optical isomers, or enantiomers, which may be either D or L isomer. Those molecules in which the configuration at the reference carbon is the same as that of D-glyceraldehyde are designated D isomers and those with the same configuration as L-glyceraldehyde are L isomers. When the hydroxyl group on the reference carbon is on the right in the projection formula, the sugar is the D isomer; when on the left, it is the L isomer. Of the 16 possible aldohexoses, eight are D forms and eight are L. Most of the hexoses of living organisms are D isomers.



D-Glyceraldehyde L-Glyceraldehyde D-Glyceraldehyde L-Glyceraldehyde

Fischer projection formulae Perspective formulae

  - Two sugars that differ only in the configuration around one carbon atom are called ***epimers***. For e.g., D-glucose and D-mannose, which differ only in the stereochemistry at C-2, are epimers, as are D-glucose and D-galactose (which differ at C-4). Some sugars occur naturally in their L form; examples are L-arabinose and the L isomers of some sugar derivatives that are common components of glycoconjugates.



D-Mannose (epimer at C-2) D-Glucose D-Galactose (epimer at C-4)

Figure 1.B.1-2
Structure of D-glucose and its two epimers i.e. D- mannose and D-galactose which differ from glucose in their stereochemistry at C-2 and C-4 respectively. Carbohydrates have been given non-systematic names, although the suffix-ose is generally used. The most common carbohydrate is glucose ($C_6H_{12}O_6$). Glucose is also called blood sugar as it circulates in the blood at a concentration of 65-110 mg/dL (or 65-110 mg/100 ml) of blood.

  - **Monosaccharides have cyclic structures** Many of the large sugar units (> C5) tend to form ring structures in solution. In aqueous solution, aldotetroses and all monosaccharides with five or more carbon atoms in the backbone occur predominantly as cyclic (ring) structures in which the carbonyl group has formed a covalent bond with the oxygen of a hydroxyl group along the chain. The formation of these ring structures is the result of a general reaction between alcohols and aldehydes or ketones to form derivatives called ***hemiacetals or hemiketals***. They contain asymmetric carbon atom and exist in two stereoisomeric forms. Six-membered rings are called ***pyranoses***, five-membered rings ***furanoses***. The open and the ring form are in equilibrium with each other. Depending on the type of monosaccharide, in aqueous solution these ring forms can be the preferred structure. Since the reaction creates an