

1 Fundamentals

1.1 Chemical bonds

1.1.1 Chemical bonds

Electrons located on the outermost shell, can escape from their atoms by supplying energy (e.g. in the form of heat) and be exchanged with other atoms. Compounds of several atoms are called molecules. The reason for the bond effort is the so-called noble gas configuration - a fulfilled valence shell - which represents an energetically stable state. Substances which have reached a full outer shell, will not form bonds (a few exceptions such as xenon-fluorine compounds are possible).

There are mainly three different types of bonds, which are discussed below.

1.1.2 The atomic bond

Nonmetals form this bond to achieve an octet of electrons. For example two fluorine atoms (each with seven outer electrons) can fill their octet of electrons by mutual exchange of one electron. The distance between the two nuclei represents a compromise between the attraction of the nuclei and the bonding electrons and the repulsion of the two nuclei and the electrons as well. The reason for the atomic bond is that nature is always striving to reach the lowest energy state. Since the electrons have more space through the bond of several atoms, which corresponds to a lower energy, the atomic bond is formed.

Since atoms try to achieve the fulfilled outer shell, elemental fluorine atoms never appear as a single atom, but always as a fluorine molecule F_2 . Also nitrogen N_2 , oxygen O_2 , chlorine Cl_2 , bromine Br_2 , and iodine I_2 . The atomic bond also is called covalent bond.

Illustration of the atomic bond of silane (SiH_4 , for silicon only the outermost shell is drawn). The silicon atom reaches the full outermost shell, the hydrogen atoms reach the filled first shell with only two electrons.

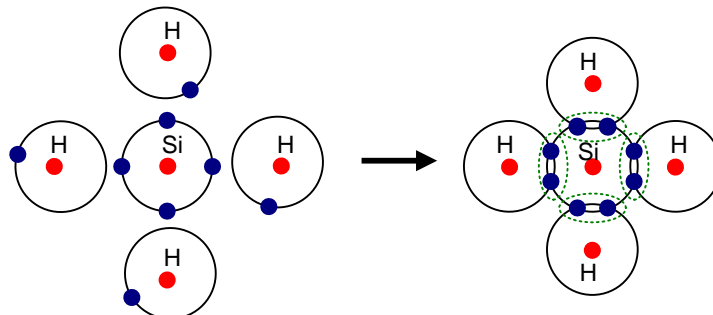


Fig. 1.1: The atomic bond of silane

1.1.3 The ionic bond

Ionic bonds are formed by the fusion of metals and nonmetals. While metals donate electrons to achieve a completely filled outer shell, nonmetals accept additional electrons. An example of an ionic bond is NaCl, sodium chloride.

The sodium atom gives off its valence electron (so it has more protons than electrons and is positively charged), while chlorine accepts one electron and thus is negatively charged. Due to the different charges the two atoms attract each other. A charged atom is known as an ion, while a positive ion is called cation and a negative ion anion, respectively.

Since atoms always occur at a very large number, they form grids due to the attraction and repulsion forces from ions. Substances which form such a grid in solid state, are known as salts.

1.1.4 The metallic bonding

Metals are forming that bond to attain the stable noble gas configuration. Each metal atom gives off its outer electrons: thus positively charged metal ions and free electrons are generated with strong attractive forces in between. The metal ions repel each other as well as the electrons.

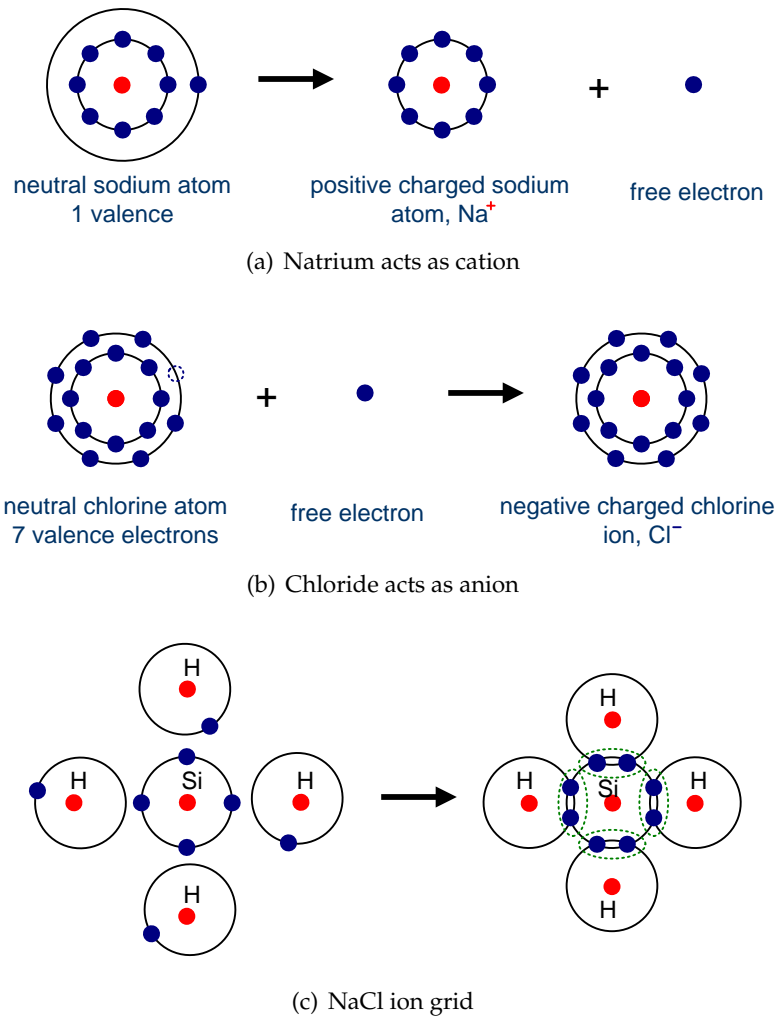


Fig. 1.2: Principle of the ion bonding

Since the attraction and repulsion forces act in all dimensions of space, the atoms arrange themselves in a regular lattice. The free electrons are the so-called Fermi gas, which holds the positive metal ions together. Due to the free electrons, metal's electric conductivity is excellent.

The physical and chemical properties of compounds are dependent on the type of bonding. Thus greater attraction forces mean higher melting and boiling points, the number of free electrons affects the conductivity.

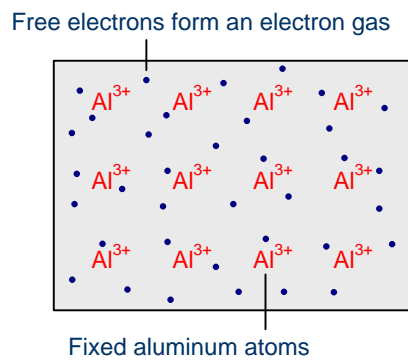


Fig. 1.3: Metallic bonding

1.1.5 Intermolecular bondings

Intermolecular bondings differ from chemical bondings in that way that these are only forces between two or more molecules, ions or atoms. Intermolecular bonds are caused mainly by load displacement which result in attracting or repulsing of particles.

The strongest of these forces is the hydrogen bond. Due to its bonding angle the loads inside a water molecule (H–O–H) are distributed asymmetrical, so that the oxygen atom has a negative partial charge while the hydrogen atoms have a positive partial charge. This load displacement leads to attracting and repulsing of other water molecules. Besides the hydrogen bond there are even weaker forces like the van der Waals interaction.

The bond energy of the chemical bonds is in the range of several hundreds to several thousands kilojoule/mol (kJ/mol). The bond energy of hydrogen bonds is up to a hundred kJ/mol and the bond energy of van der Waals forces is in the range of 0.5 to 5 kJ/mol.