

2.1: Classification of bonding

The bond in which a pair of electrons bind atoms A and B is called a covalent bond, and it is written as A-B or A:B. Since two pairs of electrons are involved in a double bond and three pairs in a triple bond, they are designated by $A=B$, $A \equiv B$ or $A::B$, or $A:::B$, respectively. The covalent bond is a simple but very useful concept proposed by G. N. Lewis at the beginning of this century and its representation is called the **Lewis structure**. Unshared pair of valence electrons are called lone pairs, and they are expressed by a pair of dots like A:.

? Exercise 2.1.1

Describe the Lewis structures of the nitrogen molecule N_2 and the oxygen molecule O_2 .

Answer

- : $N:::N$:
- : $O::O$:

Eight electrons are required to fill an s and three p orbitals, and when the total number of electrons used for the bonds and lone pairs is eight, a stable molecular structure results. This is called the **octet rule** and is useful when qualitatively discussing the molecular structures of main group compounds. Of course, this rule is not applied to a hydrogen molecule, H_2 , but is applicable to covalent molecules, such as simple two-atomic molecules O_2 or CO and even to complicated organic compounds. For the elements after the 3rd period, the number of covalent bonds is sometimes five (e.g. PCl_5) or six (e.g. SF_6), and the central atom of these molecules shows **hypervalency**. In this case, because s and p electrons run short to form more than four 2-electron covalent bonds, it was once believed that d electrons were partly involved. The present view is, however, that these hypervalent bonds use only s and p orbitals but that the bond orders are lower than those of single bonds.

The electrostatic bond between cations (positive ion) and anions (negative ion), such as in sodium chloride, $NaCl$, is called an ionic bond. Since the total electrical charge in a compound should be zero, the electrical charges of cations and anions are equal. There is a partial contribution from covalent bonds even in an ionic compound, and the ions are not necessarily bonded only by the electrostatic interaction.

Pauling's electroneutrality principle states that the net electrical charge of each component of a compound is essentially neutral. As will be mentioned later, the structures of many solid compounds are described as an alternate array of cations and anions, and are classified into several representative crystal types.

Metal atoms are bound together by means of the **conduction electrons** originating from the valence electrons of metal atoms. The bond due to the conduction electrons in a bulk metal is called the **metallic bond**.

Generally, chemical bonds can be assigned to either of the three kinds mentioned above, but new compounds have been synthesized one after another which cannot always be classified by the simple **2-center electron pair covalent bond**. They include **electron-deficient bonds** in boron hydrides, **coordinate bonds** in transition metal complexes, the **metal-metal bonds** in metal cluster compounds, etc., and new concepts have been introduced into bond theory to account for these new kinds of chemical bonds. As has already been described, a weak bonding interaction called the **van der Waals interaction** has been recognized in neutral atomic or molecular compounds. The potential of this interaction is inversely proportional to the 6th power of the distance between atoms. The adjacent but non-bonded distance between atoms is estimated by the sum of the van der Waals radius assigned to each atom.

The weak interaction X-H-Y that a hydrogen atom forms with the atoms X, Y (nitrogen, oxygen, fluoride, etc.) with larger electronegativity than that of hydrogen is called the **hydrogen bond**. Hydrogen bonding plays an important role in ice, the structure of the double helix of DNA (deoxyribonucleic acid), etc.

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