MOLECULAR ORBITALS

The nature of the chemical bond

At an elementary level, we can think about atoms being held together by simple electrostatic attraction. It is a fundamental principal that opposite charges attract. A positively charged ion and a negatively charged ion are held together by this force of attraction.

- □ This idea works well for ionic compounds, such as sodium chloride.
- It does not work well for compounds in which similar atoms are connected, such as ethane, C₂H₆.

Maybe the carbons are negatively charged and the hydrogens are positively charged, but what is holding the two carbons together if they have like charges?

A similar problem is encountered in diatomic molecules such as H₂. Is one of these hydrogen atoms negative while the other hydrogen atom is positive?

In the early twentieth century, G. N. Lewis noticed a trend in the characteristics of compounds that he called "the rule of two". If you were to count up the total number of electrons in any stable compound, you would always come up with an even number -- that is, some number that is divisible by two. Perhaps, Lewis reasoned, this predominance of even numbers arises because electrons need to be in pairs.

What does an element do if it has an odd number of electrons? One solution is to steal an electron from another element, or to allow one to be stolen away; these arrangements lead to ionic bonds. However, those elements not adept at stealing electrons may have a problem; they may need to share them instead. In order to share electrons, elements will have to form close associations with each other. They will become bonded together.

- An "ionic bond" is an electrostatic interaction between an anion and a cation.
- □ A "covalent bond" is one pair of electrons shared between two atoms.

Lewis took this idea further. If you count up the valence shell electrons around each of the atoms in stable compounds, not only are there even numbers, but there are almost always the same number of electrons as there are in one of the noble gases: He, Ne, Ar, Kr (2, 8, 8, or 18). This observation is sometimes called the Lewis octet rule because so many common atoms that form stable compounds obtain 8 electrons in their outermost shell as a result. Neon is the nearest noble gas to carbon, oxygen and nitrogen, and all of these atoms adopt 8-electron configurations in stable compounds.

Lewis structures illustrate how atoms can maintain these numbers of electrons by sharing with other atoms. These simple structural drawings are used to convey most of our ideas about molecular chemistry. However, additional information can often be found through quantum mechanics and a molecular orbital approach to bonding.

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