WHAT IS A MOLECULE?

Even at the end of the 19th century, when compounds and their formulas had long been in use, some prominent chemists doubted that molecules (or atoms) were any more than a convenient model. Molecules suddenly became real in 1905, when Albert Einstein showed that Brownian motion, the irregular microscopic movements of tiny pollen grains floating in water, could be directly attributed to collisions with molecule-sized particles.

Most people think of molecules as the particles that result when atoms become joined together in some way. This conveys the general picture, but a somewhat better definition that we will use in these lessons is

A molecule is an aggregate of atoms that possesses distinctive observable properties

A more restrictive definition distinguishes between a "true" molecule that exists as an independent particle, and an extended solid that can only be represented by its simplest formula. Methane, CH4, is an example of the former, while sodium chloride, which does not contain any discrete NaCl units, is the most widely-known extended solid.

But because we want to look at chemical bonding in the most general way, we will avoid making this distinction here except in a few special cases. In order to emphasize this "aggregate of atoms" definition, we will often use terms such as "chemical species" and "structures" in place of "molecules" in this lesson.

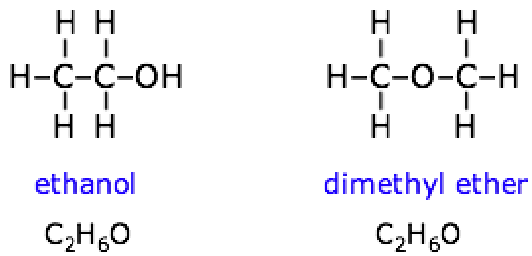
The definition written above is an operational one; that is, it depends on our ability to observe and measure the molecule's properties. Clearly, this means that the molecule must retain its identity for a period of time long enough to carry out the measurements. For most of the molecules that chemistry deals with, this presents no difficulty. But it does happen that some structures that we can write formulas for, such as He2, have such brief lives that no significant properties have been observed. So to some extent, what we consider to be a molecule depends on the technology we use to observe them, and this will necessarily change with time.

Structure, structure, structure!

And what are those properties that characterize a particular kind of molecule and distinguish it from others? Just as real estate is judged by "location, location, location", the identity of a chemical species is defined by its structure. In its most fundamental sense, the structure of a molecule is specified by the identity of its constituent atoms and the sequence in which they are joined together, that is, by the bonding connectivity.

This, in turn, defines the bonding geometry— the spatial relationship between the bonded atoms.

The importance of bonding connectivity is nicely illustrated by the structures of the two compounds ethanol and dimethyl ether, both of which have the simplest formula C2H6O. The structural formulas reveal the very different connectivities of these two molecules whose physical and chemistry properties are quite different:



Structures without molecules: stability and reactivity

The precise definition of bonding energy is described in another lesson and is not important here. For the moment you only need to know that in any stable structure, the potential energy of its atoms is lower than that of the individual isolated atoms. Thus the formation of methane from its gaseous atoms (a reaction that cannot be observed under ordinary conditions but for which the energetics are known from indirect evidence)

$$4\ H(g) + C(g) \rightarrow CH4$$

is accompanied by the release of heat, and is thus an exothermic process.

The quantity of heat released is related to the stability of the molecule. The smaller the amount of energy released, the more easily can the molecule absorb thermal energy from the environment, driving the above reaction in reverse and leading to the molecule's decomposition. A highly stable molecule such as methane must be subjected to temperatures of more than 1000°C for significant decomposition to occur. But the noble-gas molecule KrF2 is so weakly bound that it decomposes even at 0°C, and the structure He2 has never been observed. If a particular arrangement of atoms is too unstable to reveal its properties at any achievable temperature, then it does not qualify to be called a molecule.

There are many molecules that are energetically stable enough to meet the above criterion, but are so reactive that their lifetimes are too brief to make their observation possible. The molecule CH3, methyl, is a good example: it can be formed by electrical discharge in gaseous CH4, but it is so reactive that it combines with almost any molecule it strikes (even another CH3)within a few collisions. It was not until the development of spectroscopic methods (in which a molecule is characterized by the wavelengths of light that it absorbs or emits) that methyl was recognized as a stable albeit shamelessly promiscuous molecule that is an important intermediate in many chemical processes ranging from flames to atmospheric chemistry.

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