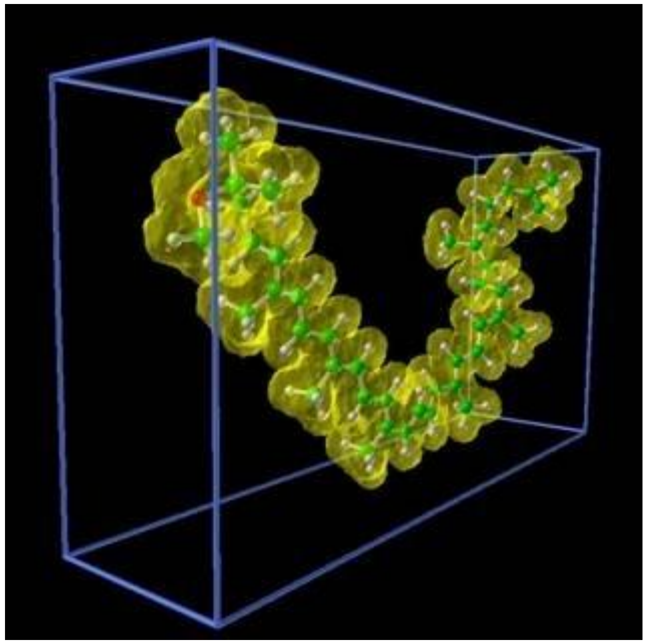
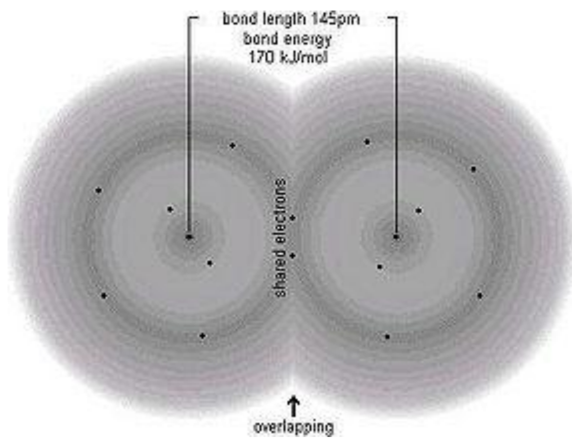
Molecule



Computer simulation of the spheroidene molecule. U.S. Department of Energy



Single bond nitrogen molecule. Source: Joseph George

A **molecule** is a stable aggregation of two or moreatoms created via a covalent bond formation by overlapping of electron clouds. Molecules are generally considered electrically neutral. Molecules can be described in terms of: (a) a molecular formula, indicating the specific combination of atoms within a given molecule; and (b) a molecular geometry incating the spatial arrangement of the atoms with respect to each other.

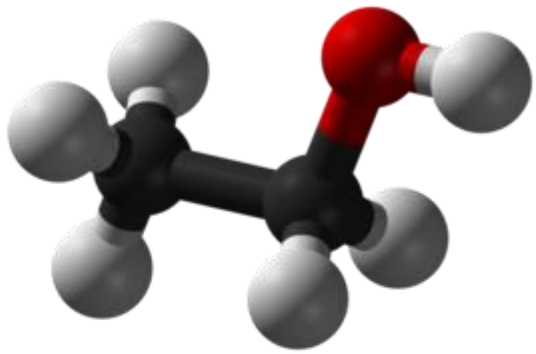
Basic concepts

A number of textbook and dictionary definitions of the term*molecule* have been challenged, such that the concept is not so simple as one might assume.[1] The notion of whether a hydrated molecule in ionized form should be considered a molecule has specifically been questioned; however, strictly speaking a dissociated molecule in solution is no longer a stable entity and thus can not be classified as a molecule. Correspondingly some dictionary definitions use the phrase *chemical force* to describe a molecule; since that term has no meaning in physics, it must be emphasized that the bond holding a molecule together is intrinsically due to an electomagnetic force. Quantum physics would, in fact, prefer to define a molecule as an aggregate of two or more atoms which has are in a state of a stable equilibrium of minimum potential energy within a space of three translational degrees of freedom. This allows for an excited state of a molecule to be classified as the same intrinsic chemical species as the molecule in its lowest state of potential energy or quantum excitation. The quantum physics view is more than an academic exercise, since the compound xenon chloride is not stable in its unexcited state and hence is only a true molecule in an excited state, as recognized by quantum physics as a minimum potential energy surface.

Over a century ago the American Chemical Society observed another problem with a classic definition of molecule, since a crystalline substance would be in its entirety considered a molecule.[2] Thus to avoid classifying such a macroscopic object as a molecule, the set of crystalline objects must be excluded from the concept of a molecule.

In certain biochemistry contexts a molecule may carry an electical charge; however, here we shall maintain a definition of electrical neutrality for the term molecule. To further complicate matters, in the kinetic theory of gases an individual atom of a noble gas is considered a gas molecule;[3] however, we will set aside that use in the treatment of molecules here.

Molecular formula



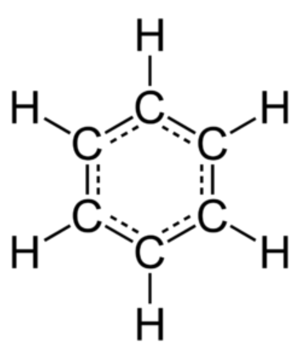
Molecular model of the ethyl alcohol molecule. Orb color codes the atom: Black (carbon); Red (oxygen); White (hydrogen)

The molecular formula is simply the designation of the molecular composition in terms of atoms present and their number. Examples of molecular formulas are:

- Water: H_2O (Two atoms of hydrogen bound with one atom ofoxygen)
- Methane: CH_4 (Four atoms of hydrogen bound with one atom of carbon)
- Oxygen: O_2: (Two atoms of oxygen bound together)
- Ethyl alcohol: C_2H_5OH or C_2H_6O (Two atoms of carbon bound with six atoms of hydrogen and one atom of oxygen)

Notice that in the case of ethyl alcohol, there are two common versions of stating the molecular formula; the method C_2H_6O is sometimes called the empirical formula, giving no information regarding the actual bonding sequence of atoms within the molecule.

Molecular structure



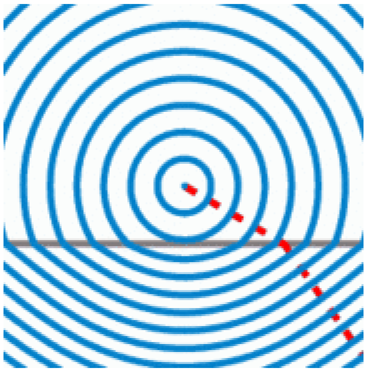
Molecular structure of benzene illustrating the hexagonal structure with carbon-carbon bond angles of 120 degrees.

Molecular structure can best be characterized by the attachment sequence of atoms, distance between adjoining atomic nuclei centers and relative angles of attachment.[4] The attachment sequence is a fundamental characteristic, since two totally different molecules with vastly different properties may have the identical molecular formula. As an example, both ethyl alcohol and dimethyl ether have identical molecular formulae (as expressed with their empirical formulas), but their molecular geometry and chemical properties are totally different; in particular, dimethyl ether has the oxygen atom bound to both carbon atoms, where ethyl alcohol has its oxygen atom bound simply to one of the carbon atoms and one hydrogen atom. The distances between nuclei centers and bond angles are viewed as intrinsic properties of a given molecule, although vibrational and rotational excitations within the molecule strictly makes these time variant, merely centered about their nominal dimensions or angles.[5]

Molecular orbitals

The concept of a molecule is inextricably linked to the existence of overlapping electron orbitals of the atoms participating in the bond. In the original formation of a given product molecule, the individual atoms or moleules coming together to form the product molecule must have their nucleii in sufficient proximity to spatially overlap the electron orbitals of the component species; in order to accomplish this approach and have the outcome be a bond between atoms, the intervening electrons must in a quantum mechanics sense be in a position to provide a net attraction to the counterpart nucleus that overcomes the inherent nuclear repulsion. When this condition is met, a new interlocked orbital can be achieved whereby the product molecule now shares at least one electron between atomic components.

Molecular properties



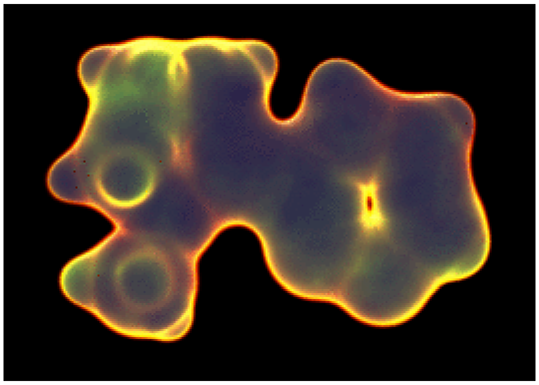
The refractive index is a property deriving from molecular structure; this video illustrates the action of waves passing between two media of differing refractive indices. Source: Oleg Alexandrov

The structure of a molecule leads inevitably to macroscopically observable properties of a given substance.[6] For example, the molecular bond gives rise to material properties that produce such measurable features as the refractive index and solubility. The most notable properties of a given molecule are:

- Color and general appearance
- Odor
- Density
- Refractive index
- Boiling and melting points
- Solubility in water and other basic solvents
- Acidity
- Electrical conductivity
- Thermal conductivity

Many of these properties are dependent on the state of matter in question (e.g. solid, liquid or gas) ortemperature and pressure at which the substance is observed.

Inorganic versus organic



Computer generated model of the nicotine molecule, a complex organic chemical.

Compounds and molecules constructed in living tissues are commonly called organic; more generally an organic molecule is one that contains the element carbon. Forms of matter not formed by living things are termed inorganic. Organisms like autotrophs usually create organic matter by consuming inorganic molecules and compounds from the lithosphere, hydrosphere, and atmosphere. An example of an autotroph is anyphotosynthesizing plant. Heterotrophs consume and assimilate other living things to create their organic matter. Herbivores and carnivores are examples of heterotrophs.

In a general sense organic chemicals include hydrocarbons, alcohols, ethers, ketones and organic acids. There are four general categories of organic compounds broadly present in living organisms: lipids, carbohydrates, proteins, and nucleic acids.

- Lipids - are composed of carbon atoms that have two hydrogen atoms attached. Lipids are commonly known as fats and oils, and belong to the family of molecules known as hydrocarbons.
- Carbohydrates - are composed of carbon, oxygen, and hydrogen atoms. Some examples are sugars, starch, and cellulose.
- Proteins - are organic compounds that are made primarily of carbon, hydrogen, nitrogen, and some other minor elements that are arranged into 20 different compounds known as amino acids.
- Nucleic Acids - are composed primarily of different combinations of carbon, hydrogen, nitrogen, oxygen, and phosphorus. They are very complex compounds being created by the atomic linking of thousands of individual atoms. DNA (deoxyribonucleic acid), the genetic blueprint of life, is an example of a nucleic acid.

History of the molecule concept

Italian scientist Amedeo Avogadro, whose work led to the recognition of molecular matter. Source: C. Sentier 1901 engraving

The concept of a molecule gained traction with Dalton's Law and Avogadro's Principle in the early 19th century. Dalton's Law states that the total pressure exerted by a mixture of gases is equal to the sum of the partial pressures of the component gases. Combined with Avogadro's work, it became generally accepted that a minute, and at that time, unobservable form of matter had to exist. Avogadro's principle states that the same number of molecules are present in a given volume of gas, regardless of the chemical nature of the gas. While this law strictly only applies to ideal gases, its approximation to real gases was so startling to scientists in the early 1800s that steady appreciation emerged of the concept of a molecular basis of gases.

The final acceptance of the concept of a molecular form of matter ensued in the latter part of the 19th century subsequent to Maxwell's treatises. Maxwell in his early work had a problem acknowledging the existence of this imperceptibly small particle. However, his work was the first to reconcile the mechanical forces known to macroscopic physics with the (then) unknown forces at the molecular level.

References

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