Cambridge University Press
978-0-521-53536-6 - Atkins' Molecules, Second Edition
Peter Atkins
Excerpt
More information

Introduction

When you hold this book you are holding molecules. When you drink coffee you are ingesting molecules. As you sit in a room you are bombarded by a continuous storm of molecules. When you appreciate the colour of an orchid and the textures of a landscape you are admiring molecules. When you savour food and drink you are enjoying molecules. When you sense decay you are smelling molecules. You are clothed in molecules, you eat molecules, and you excrete molecules. In fact, you are made of molecules.

A molecule is a characteristic grouping of atoms of the kind shown in the illustrations throughout this book. Until the beginning of the twentieth century, molecules were regarded as little more than abstract accounting symbols used by chemists to describe their reactions. However, in an extraordinary collaboration, physicists and chemists have confirmed the reality of molecules. First, they used indirect methods to infer the existence of these tiny particles of matter. Later, they used more sophisticated techniques to obtain what had long been sought – compelling images of individual molecules and atoms.

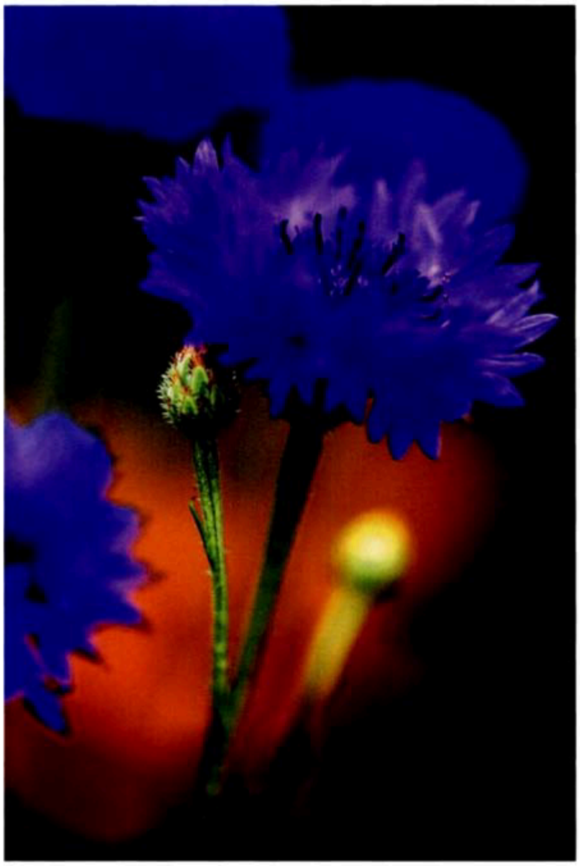
The following pages are intended to show a little of what has been found. They show the molecules we breathe, wear, eat, burn, and see all around us. The primary purpose of the illustrations is to acquaint you with their variety with a minimum of technical prerequisites. The molecules described here range from the simplest possible to the highly complex. Some do ostensibly humdrum things, such as methane (15), which is merely burned.[1] Others are included because they act as molecular building blocks, or they happen to typify a taste or an odour, or they are responsible for a colour. Some molecules do very grand things and are included here because of their importance. Among these is the most ubiquitous chemical in the world, cellulose (93), which grows as great forests and softens the face of the Earth, and deoxyribonucleic acid, DNA (203), which encodes the generations. We shall see how the replacement of one or two

---

[1] Numbers in parentheses refer to molecules described in the text.

atoms can convert a fuel into a poison, change a colour, render an inedible substance edible, or replace a pungent odour with a fragrant one. That changing a single atom can have such consequences is the wonder of the chemical world.

The illustrations alone will tell you much about the compositions and appearances of the molecules, and your perusal could, with profit, stop there. However, the drawings are enriched by knowing what they represent and understanding how a molecule performs its function. The remaining paragraphs of this introduction explain some of the background to the illustrations, suggest how to think about them, and sketch a few of the arguments that lead from atoms to molecules to properties. Chemistry provides a bridge between the familiar and the fundamental. These pages will give but a mere glimpse of this bridge but, with luck, you will see a little through the mist and understand how a chemist thinks.



A single atom can make a considerable difference to the properties of a molecule. The molecules responsible for the blue of a cornflower (*Centaurea cyanus*) and the red of a poppy (*Papaver orientale*) differ by only one hydrogen atom. This is explained in more detail on page 175.

ELEMENTS AND ATOMS

One of the great achievements of chemistry has been to show that all the matter in the world, be it a lump of rock, a glass of water, an ostrich feather, or a tree, is built from no more than a hundred or so simple substances called *chemical elements*. The elements include hydrogen, carbon, oxygen, and copper, and are so called because they cannot be broken down into simpler substances by heating, roasting, boiling, treatment with acid, or any of the other techniques that chemists use for changing matter. Physicists, of course, have developed more aggressive techniques, and they can smash elements apart into electrons, protons, and the other fundamental particles of nature using their particle accelerators. However, for our purpose, which is to explore our surroundings, we can stay with the hundred or so elements and marvel that the rich tapestry of the world can be stitched from so meagre a selection of thread.

The smallest particle of an element that can exist is an *atom* (from the Greek *atomos*, 'uncuttable'). A lump of a pure element, such as a lump of pure gold, is a collection of identical atoms; a lump of carbon is also a collection of identical atoms, but each atom is different from an atom of gold. Atoms are very small: the diameter of a carbon atom is only about 0.15 billionths of a metre (0.000 000 000 15 metres, 1.5×10^{-10} m), so a 1.5-centimetre line of carbon (about this long: ————) is a hundred million carbon atoms from end to end and about a million atoms across. Any visible lump of matter – even the merest speck – contains more atoms than there are stars in our galaxy. When we lift an apple we feel the total weight of a colossal number of almost weightless atoms. When we hear the ripple of water we are hearing shockwaves as a myriad of almost imperceptible molecules crash down and collide with other molecules. When we dress we pull across our bodies a great web spun from almost infinitesimal dots and held together by the forces acting between them. When we see a flame we are seeing the release of an almost negligible droplet of energy, but in such a Niagara that the heat sears and consumes.

Each atom consists of a very tiny central *nucleus* with a positive electric charge. That nucleus is surrounded by a sufficient number of negatively charged electrons to cancel out its charge, so the atom as a whole is electrically neutral. The electrons form a series of concentric shell-like clouds round the nucleus, so it is convenient to think of atoms as minute spheres. In this book, we represent atoms by spheres magnified up to 50 million times, so a carbon atom is represented by a sphere nearly 1 centimetre in diameter. Oxygen and nitrogen atoms have about the same number of electrons as carbon (eight and seven, respectively, in place of carbon's six) and are almost the same size as carbon atoms. A hydrogen atom is appreciably smaller because in place of carbon's six electrons it has only one. Most of the other atoms that we shall meet are appreciably larger than carbon. Phosphorus, sulfur, and chlorine atoms all have more than twice as many electrons as carbon (15, 16, and 17, respectively) and we represent them by spheres of correspondingly larger diameters.

We consider fewer than a dozen elements in this book. Each one is denoted by a chemical symbol, which is commonly the first letter of its name (with occasionally the inclusion of a later letter):

H	hydrogen	C	carbon	N	nitrogen	O	oxygen
F	fluorine	P	phosphorus	S	sulfur	Cl	chlorine

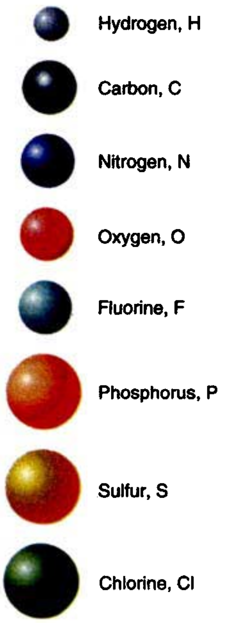
Remnants of Latin derivatives sometimes raise their head, as in Na for sodium (*natrium*), K for potassium (*kalium*), and Fe for iron (*ferrum*).

Very occasionally we shall meet the concept of an 'ion'. An *ion* is an atom that has lost or gained one or more (negatively charged) electrons and hence has acquired an electric charge. When an atom loses electrons it becomes positively charged and is called a *cation*. An example is the sodium ion, Na^+, which is a sodium atom that has lost one electron. Potassium, K, sodium's neighbour in the periodic table, can also lose an electron to form a singly charged potassium cation, K^+. A magnesium cation, Mg^{2+}, is a magnesium atom that has lost two electrons and become doubly positively charged. When an atom gains electrons it becomes negatively charged and is called an *anion*. A chlorine atom forms a singly charged chloride anion, Cl^-, by gaining one electron. An oxygen atom forms the doubly charged oxide anion, O^{2-}, by gaining two electrons. Once again, the precise number of electrons that an atom can gain or lose depends on the internal structure of its atoms, and the ions mentioned in this paragraph include most of those we need consider.

COMPOUNDS

A *compound* is a definite, fixed combination of elements. Thus, water (5) is a combination of hydrogen and oxygen, and aspirin (170) is a combination of carbon, hydrogen, and oxygen.

Many compounds consist of *molecules*, our subject. A molecule, as mentioned before, is a specific, discrete grouping of atoms in a definite geometrical arrangement. Numerous illustrations of models of molecules appear later in the book, so you can turn to almost any page to see an example. Almost all the molecules we describe consist of atoms of no more than half a dozen elements, and in many cases just two or three. That is one of the wonders of the world, that so much can be spun from so little, just as the world's literature can be spun from two dozen letters. Because we need to depict so few elements, we can distinguish between them by using spheres of different colours and will use the convention shown overleaf. These colours are commonly used, and in some cases have been chosen to allude to typical properties of the elements themselves. Thus, hydrogen is shown as white (pale grey in practice) because it is the simplest atom; carbon is as black as soot; and oxygen, the life-giver, is red. Chlorine is a greenish-yellow gas (hence, its name, The atoms of the elements shown in the illustrations later in the book are distinguished by this colour code.



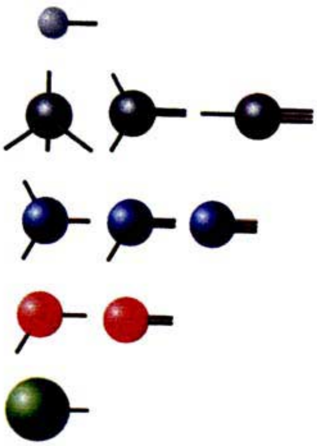
from the Greek *khloros*, ‘green’) and sulfur is a yellow solid. Just occasionally, we shall need to invoke another element and introduce it as required. Finally, we use purple spheres to represent the metal ions (specifically, sodium and potassium ions). The molecular structures based on spheres shown in the following pages are called ‘space-filling models’ because they give a reasonably accurate impression of the bulk of the molecule.

The composition of a molecule is denoted by listing the chemical symbols of the elements it contains and denoting the number of atoms of each element by a subscript (with 1 omitted). Thus, H_2O tells us that a molecule of water consists of two hydrogen atoms and one oxygen atom. The chemical formulas of the male and female sex hormones, testosterone, $C_{19}H_{28}O_2$ (195), and oestradiol, $C_{18}H_{24}O_2$ (196), show that a great deal of strife and joy, not to mention literature and warfare, stems from the difference amounting to one carbon atom and four hydrogen atoms.

BONDS BETWEEN ATOMS

The links between atoms that hold them in specific geometrical arrangements are called *bonds*. For our purposes all it is necessary to know is that a chemical bond is a shared pair of electrons. This idea,

Cambridge University Press
978-0-521-53536-6 - Atkins' Molecules, Second Edition
Peter Atkins
Excerpt
More information



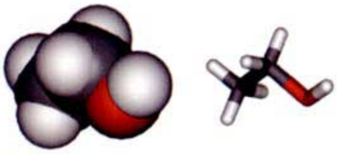
The atoms of the elements form characteristic numbers of bonds as shown here.

which was first proposed by the American chemist G. N. Lewis in the opening decades of the twentieth century, has survived the rigours of quantum-mechanical scrutiny with only minor changes of detail. We can picture a bond as two electrons that hover between the nuclei of the atoms they join and act as a kind of electrostatic glue.

The number of bonds that a given atom can form is a reflection of the number of electrons it can share with its neighbours. The rules governing this ability, which can be explained by going further into atomic structure, are as follows:

- a hydrogen atom usually forms only one bond
- a carbon atom usually forms four bonds
- a nitrogen atom usually forms three bonds
- an oxygen atom usually forms two bonds
- a chlorine atom usually forms one bond.

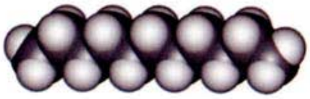
In writing the *structural formula* of a molecule, a depiction of the bonding pattern in a molecule, a bond is represented by a short single line (–) between the chemical symbols of the atoms it joins. The bond between a hydrogen atom and a chlorine atom in hydrogen chloride, HCl, is therefore represented as H–Cl. Because the arrangement of atoms in models of complex molecules is often difficult to make out, we shall also include *tube structures* or 'stick' structures showing the bonding pattern alone, with the tubes representing the bonds coloured at each end to indicate the identity of the element using the same code as for the 'space-filling' spheres. Thus, an ethanol molecule can be represented as



The illustration on the left is a space-filling model and that on the right is a tube structure.

Some atoms can form more than one bond to another atom. When a carbon atom shares two pairs of electrons with a neighbouring oxygen atom, for example, there is a *double bond* between them. This double bond is denoted C=O, and it can be seen in many of the structures shown later, including acetic acid (31) and testosterone (195). Similarly, two atoms can share three pairs of electrons, in which case the atoms are joined by a *triple bond*, as in the hydrogen cyanide molecule H–C≡N (115).

Single bonds act like hinges, because one end of the molecule can be twisted relative to the other end of the molecule, so molecules can coil into many different shapes. Although we might show a chain of carbon atoms laid out in a straight line, as in



we should think of the chain as ceaselessly writhing and wriggling and adopting shapes like

and

Where the two parts of a molecule are joined by a double bond that ability to coil is lost because one end of the molecule cannot rotate relative to the other around the torsionally rigid double bond.

ORGANIC COMPOUNDS

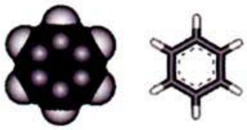
Most of the compounds shown in the following pages are *organic*. That is, they are compounds containing carbon and (usually) hydrogen. Compounds that are not organic are called *inorganic*. Some very simple carbon compounds, particularly those not containing hydrogen (carbon dioxide, chalk, and other carbonates, for example) are honorary inorganic compounds.

The term 'organic' does not mean that the compounds are necessarily made by biological organisms, although that was once thought to be the case and is the origin of the name. It was once believed that organic compounds contained some kind of 'vital force' that led to life. That view was overturned in the nineteenth century, when it was shown that a typical organic compound, urea (147), a component of urine, could be made from inorganic starting materials.

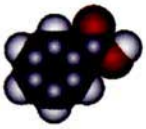
Organic compounds are prominent in these pages because they are so important and interesting. They are responsible for the colours and odours of flowers and vegetation and for the taste of food. Indeed, virtually the whole of the natural world, apart from the rocks and the oceans, consists of organic compounds. Many of the newer construction materials, notably plastics, are also organic, as are almost all pharmaceuticals.

Carbon, through the organic compounds it forms, plays a special role in the world because it has a unique ability to form bonds with itself. A glance at the following pages will show many examples of molecules that consist of chains and rings of black carbon spheres. A few other elements can link to themselves (sulfur among them), but none so extensively as carbon, and none gives so many stable structures. Carbon has this unique ability because it is rather mediocre and undemanding as an element. It has a middling ability to attract electrons from other atoms, and its own electrons can be removed fairly easily. In other words, it is promiscuous in its ability to share electrons, and can therefore form a huge number of liaisons.

When looking at the organic molecules pictured in the following pages, it is often helpful to think of them as chains or rings of carbon atoms that form an underlying framework. With the framework in mind, the structure of the molecule can be identified by noting the other groups of atoms that are attached to it. For example, a common structural motif is the hexagonal benzene ring:



The dashed line inside the hexagon on the right indicates that the double-bond character of the bonding between three pairs of carbon atoms is shared equally around the ring. A molecule derived from benzene is benzoic acid, a benzene ring to which the 'carboxyl group', –COOH, is attached:



The commonly occurring groups, such as –COOH, that decorate basic frameworks are called *functional groups* and are often the chemically active parts of organic molecules. Examples of functional groups that occur frequently in the molecules we consider are the hydroxyl group, –OH, the carbonyl group ($>C{=}O$), and the carboxyl group (–COOH).

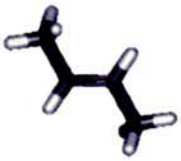
Another feature to which we must be alert is the fact that the same molecular formula may apply to two or more different substances because the same atoms can be linked in a variety of ways, each bonding pattern corresponding to a different compound. An example is the molecular formula C_2H_6O, which applies both to ethanol and to dimethyl ether:

Ethanol, C_2H_6O

Dimethyl ether, C_2H_6O

Different compounds with the same molecular formula are called *isomers*, from the Greek for 'equal parts', as the different molecules can be thought of as built from the same kit of atoms. These two isomers, ethanol and dimethyl ether, differ in the 'connectivity' of the molecules, which atom is joined to which. Another kind of isomerism occurs when two molecules have the same atoms joined together (that is, have the same connectivity) but differ in the arrangement of those atoms in space. This *geometrical isomerism* is illustrated by the following two compounds of composition C_4H_8:

cis-2-Butene



trans-2-Butene