Chapter 15

WHY ARE THERE SO MANY CARBON COMPOUNDS I?

Up to this chapter, the focus has been on inorganic compounds. Yet of the millions of known chemical compounds, the vast majority are organic compounds. In this chapter, the variety of compounds containing just carbon and hydrogen will be discussed.

15.1 Background

Before 1828, any substance that was isolated from animal or plant material was thought to contain some kind of "vital force." This theory of vitalism suggested that substances found in living organisms could not be prepared in a laboratory and they were given a separate category of "organic" compounds – in contrast to those obtained from rocks and minerals which were named "inorganic."

It was in 1828 that the German chemist, Friedrich Wöhler, tried to prepare the compound ammonium cyanate by a double replacement reaction. The cyanate ion, CNO^-, is like the cyanide ion, but with an oxygen atom attached. Wöhler reacted silver cyanate solution and ammonium chloride solution, hoping for a double replacement reaction to give a solution of the desired compound, ammonium cyanate:

$$AgCNO(aq) + NH_4Cl(aq) \rightarrow AgCl(s) + NH_4CNO(aq)$$

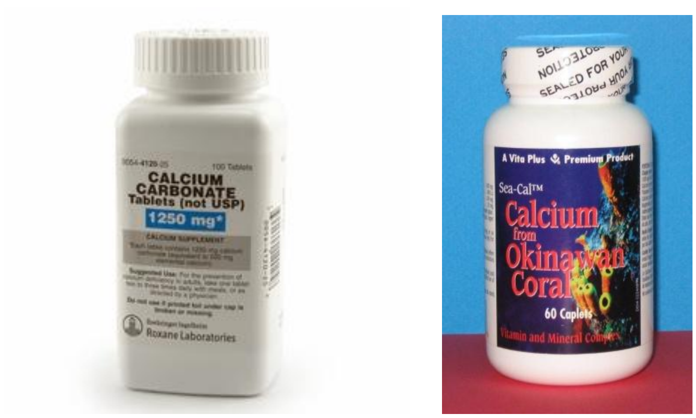
Figure 15.1 A postage stamp issued to commemorate the discovery by Friedrich Wöhler of a chemical reaction which converted an inorganic compound to an organic compound.

Wöhler filtered off the insoluble silver chloride, then he gently heated the solution of ammonium cyanate, evaporating the water, in the anticipation of producing crystals of the compound. To his amazement, the crystals formed were not those of ammonium cyanate, but of an already known "organic" compound, called urea, $CO(NH_2)_2$. Both compounds have the same molecular formula, but the effect of warming had caused the atoms in the ionic ammonium cyanate to rearrange to produce a compound containing only covalent bonds.

$$NH_4CNO(aq) \xrightarrow{\Delta} CO(NH_2)_2(aq)$$

Up until then, urea had only been obtained from urine. This single experiment showed that there was no difference between a compound synthesized in the laboratory and one of the same formula and structure found in nature.

Unfortunately, nearly 200 years later, many people are fooled by claims that so-called "natural" products are in some way more beneficial than the identical chemical compound synthesized in a chemical laboratory (Figure 15.2).



(a) (b)

Figure 15.2 Calcium carbonate that is laboratory-synthesized (a) and calcium carbonate that is from coral reefs (b) consists of identical Ca^{2+} cations and CO_3^{2-} anions.

15.2 The Differences Between Organic and Inorganic Compounds

Organic compounds can be defined as the chemistry of carbon compounds. There are a few exceptions, in that simple carbon-containing compounds, such as carbon monoxide, carbon dioxide, and hydrogen cyanide are classified as inorganic. The polyatomic ions, carbonate and cyanide, are also considered inorganic.

Whereas many inorganic compounds contain ionic bonds, almost all organic compounds contain only covalent bonds. One significant chemical difference between organic compounds and most inorganic compounds is that organic compounds will burn in the oxygen of the air. This is the reason why fuels for heating – wood, gas, oil, coal – are all carbon-based. Such reactions are called combustion reactions and the products from complete combustion are mostly carbon dioxide and water vapour. As an example, here is the reaction for the combustion of methane (natural gas):

$$CH_4(g) + 2\ O_2(g) \rightarrow CO_2(g) + 2\ H_2O(g)$$

The key differences between inorganic and organic compounds are shown in Table 15.1 below:

Table 15.1 A comparison of inorganic and organic compounds

Inorganic	Organic
Often contain ionic bonds	Contain covalent bonds
Usually have simple formulas with only a few atoms	Often have complex formulas with many atoms
One formula usually represents a unique compound	One formula can represent many different compounds

It was mentioned in Chapter 10, Section 10.5 Group 14, that carbon is a unique element in that carbon atoms can covalently-bond together to form chains – an ability called catenation. As a result of carbon atoms being able to link together in many different ways, as will be shown in subsequent sections, there can be many compounds with the same molecular formula. For example, there are three different compounds with the molecular formula C_5H_{12}; 75 compounds with the molecular formula $C_{10}H_{22}$; and 366,319 compounds with the formula $C_{20}H_{42}$.

15.3 The Shapes of Organic Molecules

Molecules are three-dimensional, whereas our writing and display surfaces are two-dimensional. Thus visualization is a key point in the study of organic chemistry – to see a flat diagram on a screen or paper and imagine it as a three-dimensional object. Adding to the complexity, carbon atoms most often forms four covalent bonds. These bonding directions are at equal angles. As can be deduced mathematically, that bond angle will be $109\frac{1}{2}^{o}$ - not a common angle!

In Chapter 6, Section 6.8, the topic of the shapes of simple molecules was introduced. The focus at that point was on the shapes of ammonia and water, and the influence of lone pairs on the molecular shape. With carbon chemistry, we are concerned with the bond angles around a central singly-bonded carbon atom and how the molecular structure can be depicted. In addition, it will be shown how the bond angle, and hence the shape, changes around the carbon atom as the bond changes from single, to double, to triple.

TYPES OF MODELS

In Chapter 6, Section 6.8, it was shown that molecules could be visualized in two different ways: space-filling models and ball-and-stick models. Space-filling models are as close as possible to how we visualize the molecule would appear, if it were possible to see it. The simplest example for carbon is the methane molecule, CH_4 (Figure 15.3). As can be seen from the Figure, the spheres representing the atoms merge together. This overlap results from the shared electron pairs in the covalent bonds.

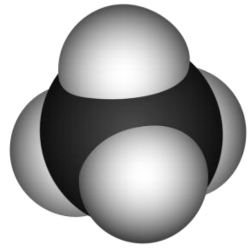


Figure 15.3 A space-filling model of the methane molecule, CH_4.

Though space-filling models provide a nice visual image of the molecule, it is impossible to see the bond angles or the number of covalent bonds. This latter point becomes important when molecules with double or triple bonds are discussed. For this reason, chemists often use ball-and-stick models. Figure 15.4 shows the methane molecule depicted as a ball-and-stick model. In most examples in this Chapter, and in Chapter 16, both images will be displayed.

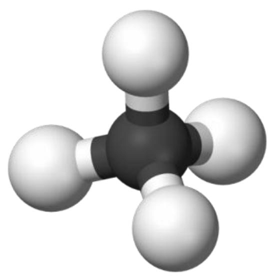
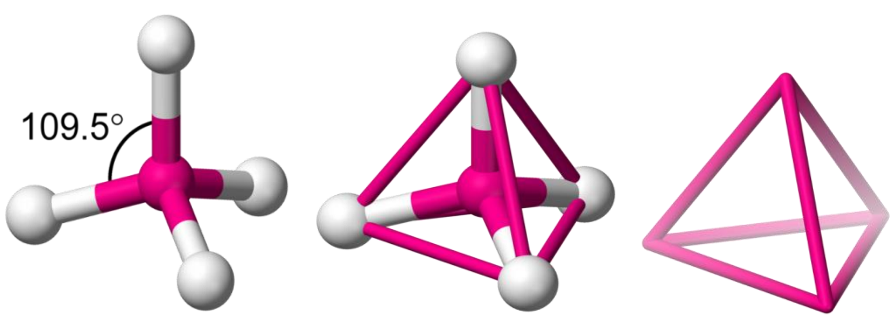


Figure 15.4 A ball-and-stick model of the methane molecule, CH_4.

The arrangement of four equal-angle bonds around the carbon atom is said to be ***tetrahedral***. A tetrahedron is a geometric shape having four triangular faces. It is possible to see why the bond arrangement is called tetrahedral in Figure 15.5.



(a) (b) (c)

Figure 15.5 (a) A ball-and-stick representation of the methane molecule (b) Constructing lines between the hydrogen atoms (c) Removing the molecule from the framework, the tetrahedron can be seen.

TWO-DIMENSIONAL REPRESENTATIONS OF ORGANIC MOLECULES

Though it is easy to display three-dimensional depth using computer-generated models, it is harder to do when drawing molecular shapes on paper. For simple molecules, ***wedge-and-dash diagrams*** can be drawn. The molecular diagram is oriented so that two C–H bonds are in the plane of the screen/paper. These two bonds are represented as lines. The C–H bond sticking out of the surface is represented as a wedge, while the C–H bond going into the screen/paper is represented as a dashed line. The diagram for methane is shown in Figure 15.6.

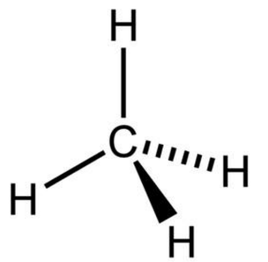


Figure 15.6 The wedge-and-dash representation of the methane molecule.

For more complex organic molecules, the depiction of the tetrahedral angles becomes more and more difficult. To simplify further, it is common to draw the molecules as ***2-D projection formulas*** or more commonly, ***structural formulas***. In these diagrams, it is imagined that the three-dimensional molecule is oriented so that its shadow on a flat surface gives equal bond angles of 90º (even though, in reality, the bond angles are $109\frac{1}{2}$º). This process is illustrated in Figure 15.7.

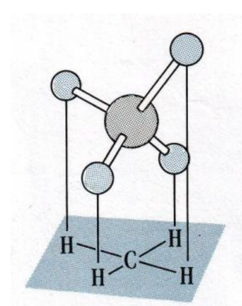


Figure 15.7 The projection of a ball-and-stick three-dimensional methane molecule onto a plane surface.

Thus the methane molecule will appear as in Figure 15.8, with all equal angles.

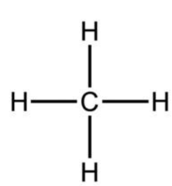
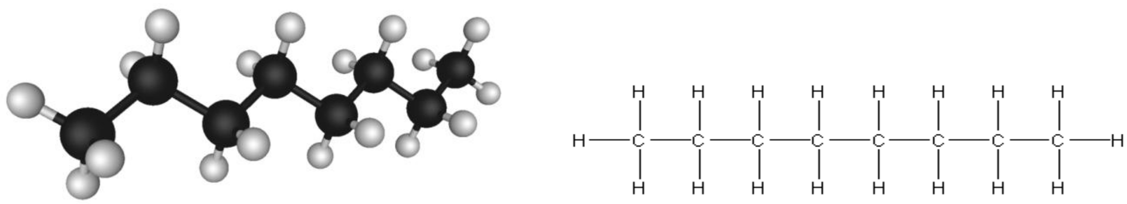


Figure 15.8 The 2-D projection formula or structural formula for methane.

It is much easier to draw a structural formula than the ball-and-stick model. To illustrate, Figure 15.9 shows, side-by-side, the ball-and-stick model and the structural formula for one of the isomers of C_8H_{18} (Figure 15.9).



(a) (b)

Figure 15.9 (a) the ball-and-stick model for an isomer of C_8H_{18} (b) the 2-D projection formula or structural formula for C_8H_{18}.

For large molecules, drawing even the structural formulas is time-consuming. Thus an even more compact representation is that of the condensed formula. In a ***condensed formula***, the number of hydrogen atoms attached to each carbon atom is simply listed following that carbon atom. For example, the condensed formula for C_8H_{18} will be represented as shown in Figure 15.10.

$$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$$

Figure 15.10 The molecule C_8H_{18} represented as a condensed formula.

15.4 Classes of Hydrocarbons

The compounds containing only hydrogen and carbon are called ***hydrocarbons***. There are two classes of hydrocarbons, aromatic and aliphatic. In ***aromatic compounds***, there are rings of carbon atoms with particularly strong carbon-carbon bonds. Section 15.12 will introduce aromatic compounds. The other class, the majority of hydrocarbons, is that of ***aliphatic compounds***. Aliphatic compounds, in turn can be categorized as ***alkanes***, in which all the carbon-carbon bonds are single bonds; ***alkenes***, in which at least one of the carbon-carbon bonds is a double bond; and ***alkynes***, in which at least one of the carbon-carbon bonds is a triple bond. The relationship between these categories is shown in Figure 15.11.

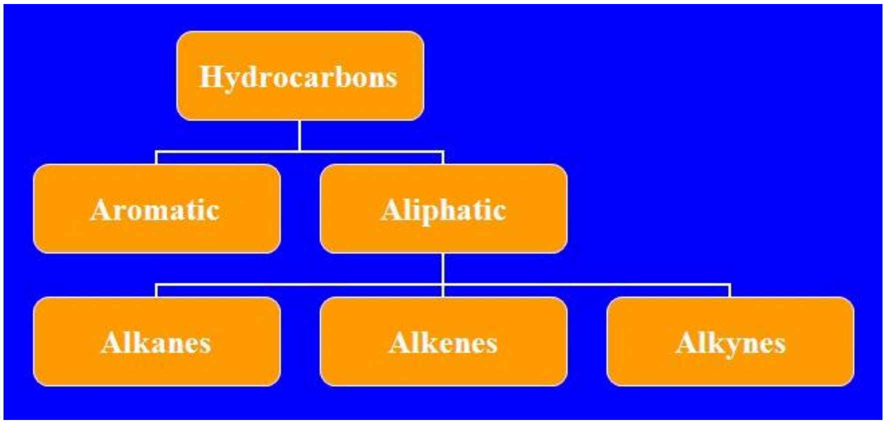


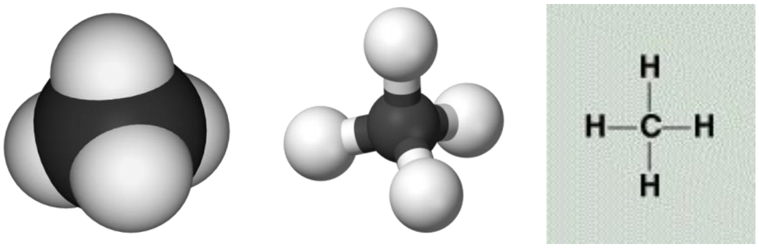
Figure 15.11 The categories of hydrocarbons.

15.5 Alkanes

As mentioned above, alkanes have only carbon−carbon single bonds. Their formulas belong to the series C_nH_{2n+2} where n is an integer from one to near infinity. Thus the formulas of the first five members will be: CH_4, C_2H_6, C_3H_8, C_4H_{10}, and C_5H_{12}.

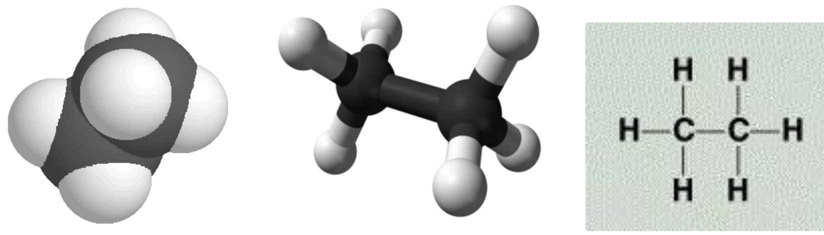
Representations of Simple Alkanes

In the first part of this Section, the representations of three simplest alkanes, CH_4 (Figure 15.12); C_2H_6 (Figure 15.13); and C_3H_8 (Figure 15.14) are depicted as space-filling and ball-and-stick models and as structural formulas. It is an important skill to realize that each of the three images represents the molecule. The space-filling model is how we imagine that the molecule might look, if we could see it. The ball-and-stick model enables us to see how the bonds are arranged. And finally, the structural formula is how we (incorrectly) display the three-dimensional molecule on a two-dimensional surface.



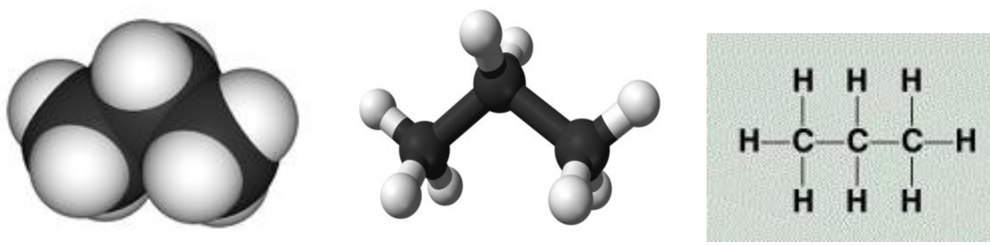
(a) (b) (c)

Figure 15.12 The CH_4 molecule represented as (a) a space-filling model, (b) a ball-and-stick model, and (c) a structural formula.



((a) (b) (c)

Figure 15.13 The C_2H_6 molecule represented as (a) a space-filling model, (b) a ball-and-stick model, and (c) a structural formula.

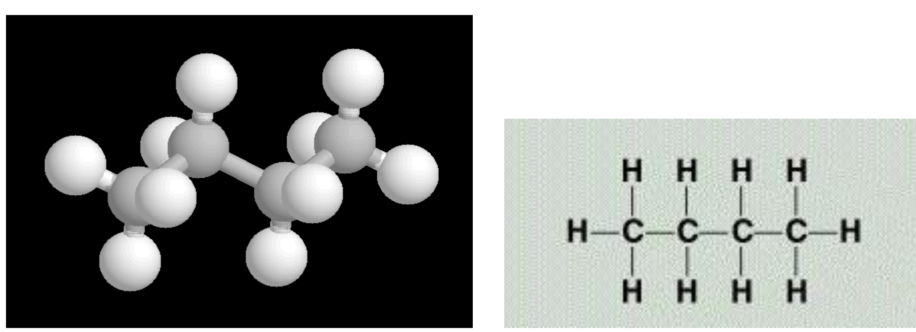


((a) (b) (c)

Figure 15.14 The C_3H_8 molecule represented as (a) a space-filling model, (b) a ball-and-stick model, and (c) a structural formula.

STRUCTURAL ISOMERS

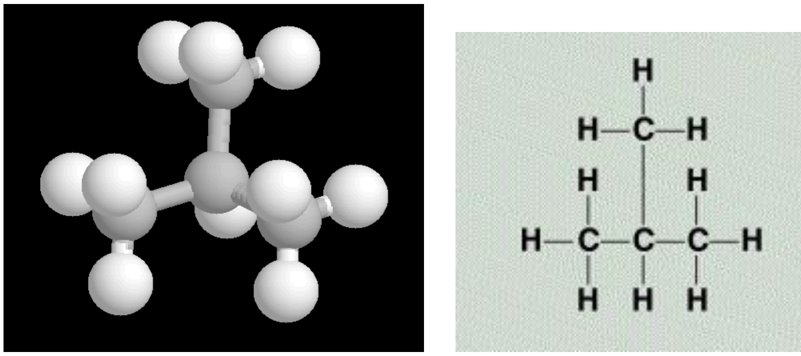
With C_4H_{10}, there are two ways in which the carbon chain can be organized. One isomer has the four carbon atoms in a row (Figure 15.15). When all the carbon atoms are in a line, it is said to be a ***straight-chain*** molecule.



(a) (b)

Figure 15.15 The straight-chain isomer of the C_4H_{10} molecule represented as (a) a ball-and-stick model, and (b) a structural formula.

In the second isomer, one of the carbon atoms is attached to the middle carbon atom of a three carbon atom chain (Figure 15.16). This is a ***branched-chain molecule***.



(a) (b)

Figure 15.16 The branched-chain isomer of the C_4H_{10} molecule represented as (a) a ball-and-stick model, and (b) a structural formula.

These two different forms are said to be structural isomers. ***Structural isomers*** occur when, for the same molecular formula, the atoms can be arranged in different ways. As the number of carbon atoms increase, the number of structural isomers of alkanes increases very rapidly as can be seen from Table 15.2.

Table 15.2 The dependence of the number of structural isomers on the number of carbon atoms

Number of carbon atoms	Number of structural isomers
1	1
2	1
3	1
4	2
5	3
6	5
7	9
8	18
9	35
10	75
12	355
15	4347

NAMING ALKANES

As was mentioned in Chapter 7, Section 7.2 Overview, the naming of organic compounds follows a different set of rules to those used for the naming of inorganic compounds. In this Chapter, the naming rules for alkanes will be covered, then later Sections will cover how these same rules can be used for other types of hydrocarbons.

The names of all alkanes have the suffix (ending) ***–ane***. The prefix represents the number of carbons in the chain. The list of prefixes corresponding to a specific number of carbon atoms is listed in Table 15.3.

Table 15.3 Prefixes used for Naming Organic Compounds of up to 10 carbon chain length

# of atoms	Prefix		# of atoms	Prefix
1	Meth-		**6**	Hex-
2	Eth-		**7**	Hept-
3	Prop-		**8**	Oct-
4	But-		**9**	Non-
5	Pent-		**10**	Dec-

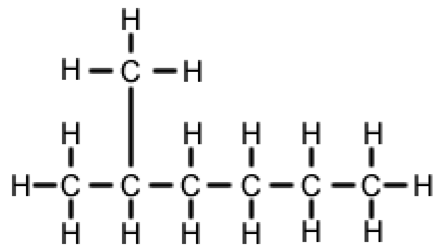
Thus the compound, C_7H_{16}, would be named heptane. However, as was illustrated in Figure 15.16, there are also branched-chain alkanes. In order to name these, additional rules must be used. The full set of rules is listed below.

1. The prefix of the name is derived from the number of carbon atoms in the longest chain.
2. To indicate that all the carbon-carbon bonds are single bonds, the suffix *–ane* is added.
3. The name of any side-groups (substituents) is placed first, using the same naming system but with the ending *–yl*.
4. The number of the carbon atom on the longest chain to which the substituent is linked is indicated by a numerical prefix.

Thus the molecule shown in Figure 15.16 has a three-carbon longest chain, hence the stem name will be "propane." There is a one-carbon side group, thus the name will be methylpropane. And normally, the number of the carbon atom on the backbone to which the side-group is attached will be included: "2-methylpropane." In this case, as there can be no other branched-chain isomer, it is acceptable to simply say "methylpropane."

EXAMPLE 15.1

Provide the IUPAC name for the following alkane:

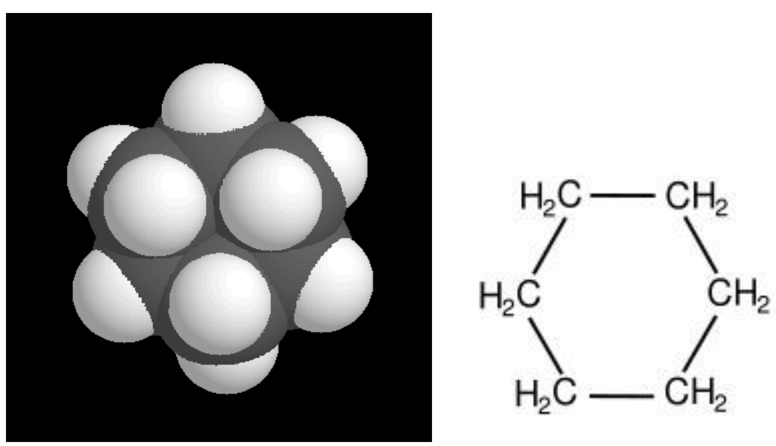


Answer

The longest chain has six carbon atoms, hence this will be named “hexane.”
In addition, there is a side methyl group, giving the name “methylhexane.”
The methyl group is located on the second carbon in the chain, thus the complete name is: *2-methylhexane*.

CYCLO-ALKANES

In addition to carbon atoms forming chains, it is possible for the ends of the chain to be removed to make a ring structure. As it is necessary to remove one hydrogen atom from the carbon atom on each end of the chain, the resulting ***cyclo-alkanes*** follow a slightly different generic formula of C_nH_{2n}. One such example is C_6H_{12} (Figure 15.17).



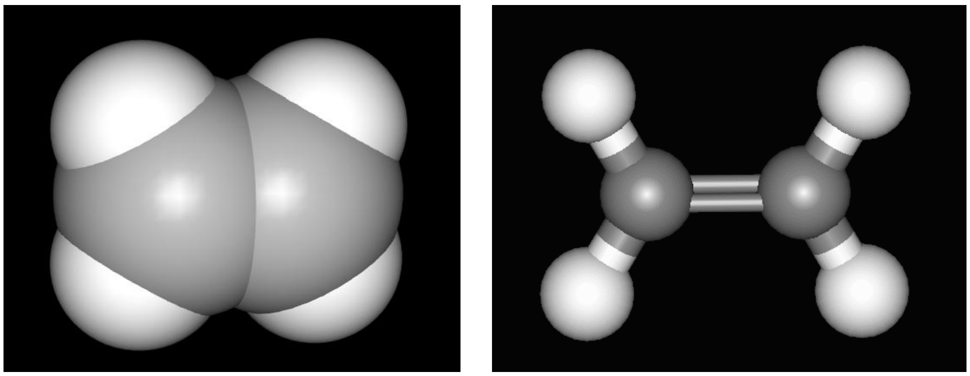
(a) (b)

Figure 15.17 The cyclic alkane, C_6H_{12}, molecule represented as (a) a space-filling model, and (b) a structural formula.

To name a *cyclo*-alkane, the same rules apply as naming straight-chain alkanes except the prefix *cyclo-* is added. Thus cyclic C_6H_{12} is named cyclohexane.

15.6 Alkenes

A hydrocarbon possessing at least one carbon-carbon double bond is called an ***alkene***. The generic formula for an alkene with only one carbon-carbon double bond is C_nH_{2n} (the same as that for a cyclo-alkane). The simplest alkene has the formula C_2H_4 and representations of the molecule are shown in Figure 15.18.



(a) (b)

Figure 15.18 The simplest alkene, C_2H_4, molecule represented as (a) a space-filling model, and (b) a ball-and-stick model.

For alkanes, there is rotation about each of the bonds, but the double bond in an alkene is rigid. The carbon atoms involved in the double bond have bonds at angles of 120° in a planar arrangement (Figure 15.19).

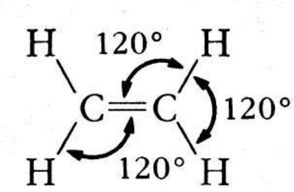
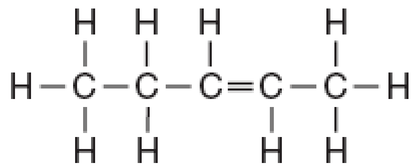


Figure 15.19 The simplest alkene, C_2H_4, molecule represented as a structural formula

NAMING ALKENES

Alkenes are named in the same way as alkanes, except the suffix is ***–ene***. The carbon chain has to include the double bond even if it is not the longest chain. In addition, the location of the lower-number carbon atom at which the double bond starts is identified by a numerical prefix.

EXAMPLE 15.2
Provide the IUPAC name for the following alkene:



Answer
The longest chain has five carbon atoms (and the chain contains the double bond), thus the name will be 'pentene.' To obtain the lower number for the location of the double bond, in this case, the count must be from right to left. Thus the full name will be ***2-pentene***.

CIS-TRANS **(GEOMETRIC) ISOMERS**
In the illustration for Example 15.2, the alkene is shown in linear form, even though there is a 120° bond angle at each end of the double bond as shown in Figure 15.19. In fact, the rigidity of the carbon-carbon double bond means that there is a second form of isomerism possible, cis-trans or geometric isomerism. This form of isomerism is unique to alkenes. The simplest example of cis-trans isomerism is found for butene, C_4H_8 (Figure 15.20).

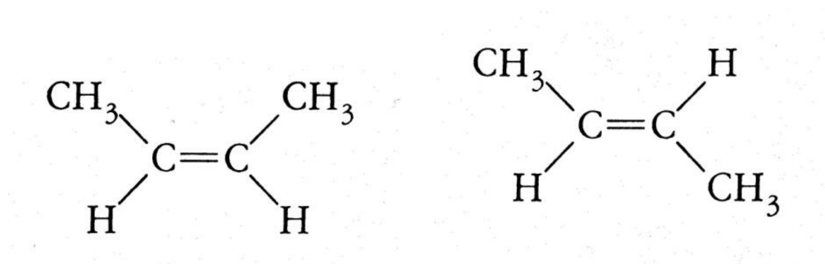
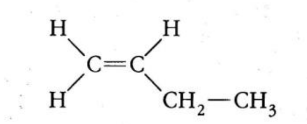


Figure 15.20 The two *cis-trans* isomers of butene (a) the *cis* isomer and (b) the *trans* isomer

Thus in naming alkenes, in addition to identifying the location of the carbon-carbon double bond, it is also necessary to identify whether it is the *cis*- or *trans*- isomer if such two different forms can occur. The *cis*- isomer is the molecule having the longest continuous chain on the same side of the carbon-carbon double bond (Figure 15.20a). This molecule would be named *cis*-2-butene. The *trans*- isomer is the molecule having the longest continuous chain on opposite sides of the double bond (Figure 15.20b). This molecule would be named *trans*-2-butene.

EXAMPLE 15.3
Will 1-butene exhibit geometrical isomerism?

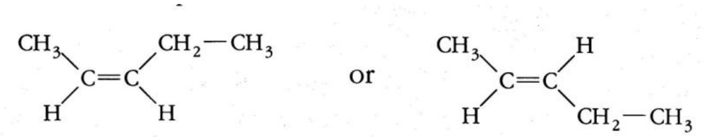
Answer
The condensed formula for 1-butene is:



As one of the carbon atoms involved in the double bond has the same species (two hydrogen atoms) attached to it, geometric isomerism cannot occur.

EXAMPLE 15.4
Will 2-pentene exhibit geometrical isomerism?

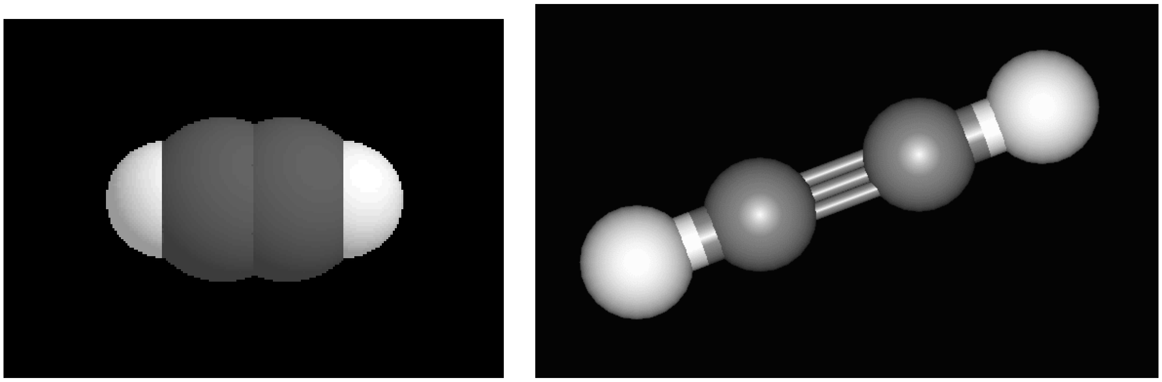
Answer
The condensed formula for 2-pentene can be drawn as:



As each of the carbon atoms involved in the double bond has different species attached to it (one methyl group and one hydrogen atom for one carbon atom; one ethyl group and one hydrogen atom for the other carbon atom), geometric isomerism can occur.

15.7 Alkynes

A hydrocarbon possessing at least one carbon-carbon triple bond is called an ***alkyne***. The generic formula for an alkyne with only one carbon-carbon triple bond is C_nH_{2n-2}. The simplest alkyne has the formula C_2H_2 and representations of the molecule are shown in Figure 15.21.



(a) (b)

Figure 15.21 The simplest alkyne, C_2H_2, molecule represented as (a) a space-filling model, and (b) a ball-and-stick model.

The bonds to each carbon involved in the triple bond are linear, that is, the bond angle is 180° as shown in Figure 15.22.

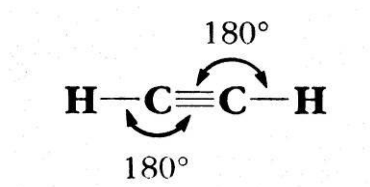


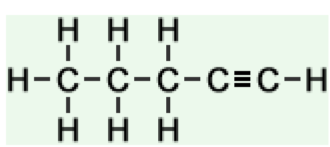
Figure 15.22 The simplest alkyne, C_2H_2, molecule represented as a structural formula

Naming Alkynes

Alkynes are named in the same way as alkenes, except the suffix is ***–yne***. The carbon chain has to include the triple bond even if it is not the longest chain. In addition, the location of the lower-number carbon atom at which the triple bond starts is identified by a numerical prefix.

Example 15.5

Provide the IUPAC name for the following alkyne:



Answer

The longest chain has five carbons, thus the name will be 'pentyne.' To obtain the lower number for the location of the double bond, in this case, the count must be from right to left. Thus the full name will be *1-pentyne*.

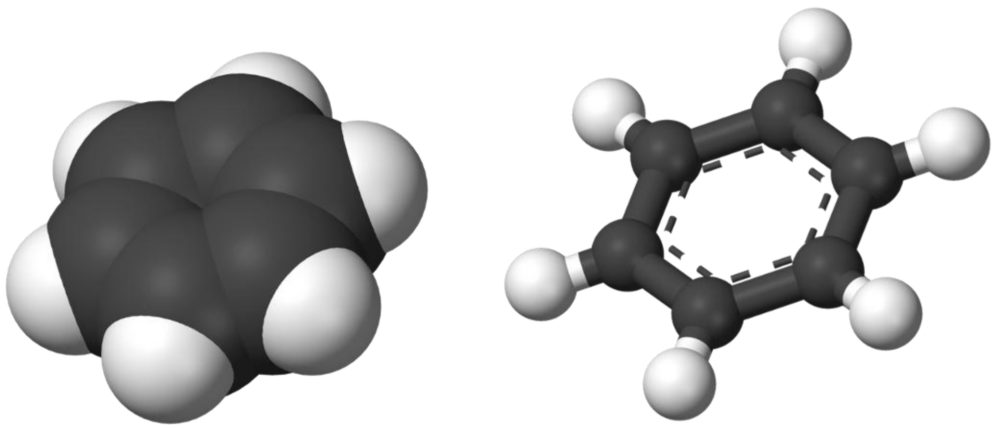
15.8 Aromatic Hydrocarbons

In Section 15.5, cyclic alkanes were discussed. It is also possible to synthesize cyclic alkenes and even cyclic alkynes. All of these behave just like the linear analogue, for example, a cyclo-alkene has much the same physical and chemical properties as a chain alkene.

However, if the ring (more specifically, a six-member ring) contains alternating single and double bonds, the compounds have unique properties. It is found that the molecule does not, in fact, contain alternating single and double bonds. Instead, each carbon-carbon bond is identical and behaves as if they are one-and-one-half bonds. More than that, the ring itself has unique properties, being much less chemically reactive than cyclic aliphatic compounds. Such compounds are called ***aromatic hydrocarbons***, as many of those first discovered had a sweet aroma.

BENZENE

The simplest common aromatic compound has the common name of benzene and its formula is C_6H_6. The two model representations of benzene are shown in Figure 15.23.



(a) (b)

Figure 15.23 The most common aromatic molecule, C_6H_6, represented as (a) a space-filling model, and (b) a ball-and-stick model.

In the structural formula, the best way to represent the $1\frac{1}{2}$ bond between pairs of carbon atoms is to use one solid and one broken line (Figure 15.24).

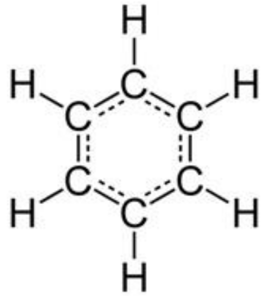


Figure 15.24 The most common aromatic molecule, C_6H_6, represented as a structural formula.

METHYLBENZENE (TOLUENE)

The closest relative of benzene is methylbenzene, commonly called toluene. The methylbenzene molecule has the same six-member ring structure of benzene, but with a methyl group in place of one of the hydrogen atoms. The space-filling model and the structural formula of toluene are shown in Figure 15.25.

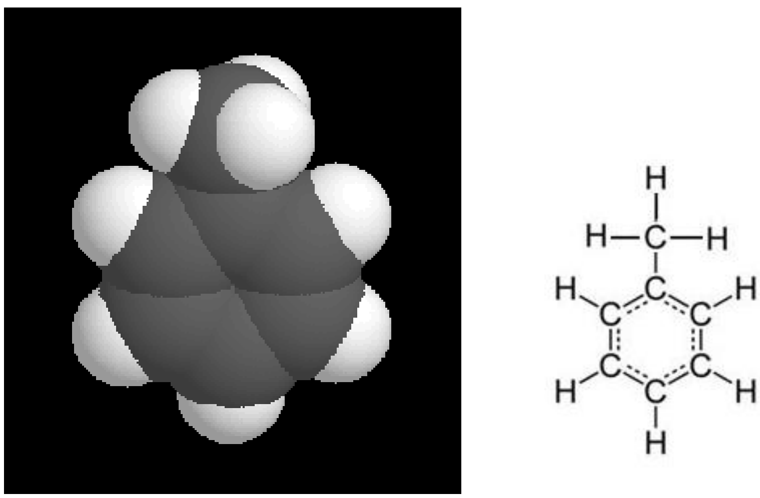


Figure 15.25 The aromatic molecule, C_7H_8, methylbenzene (toluene), represented as (a) a space-filling model, and (b) a structural formula.

POLYCYCLIC AROMATIC HYDROCARBONS

In addition to single aromatic rings, it is possible for aromatic compounds to have multiple rings. Many of these ***polycyclic aromatic hydrocarbons*** (abbreviated to PAHs) – particularly with three, four or even more rings joined together are carcinogenic. They are found in the environment mainly as a product of combustion, such as smoke from wood-burning stoves and on char-broiled foods.

The simplest PAH is naphthalene, $C_{10}H_8$, which is sometimes used to kill moths in clothes storage locations. The space-filling and ball-and-stick models of naphthalene are shown in Figure 15.26.

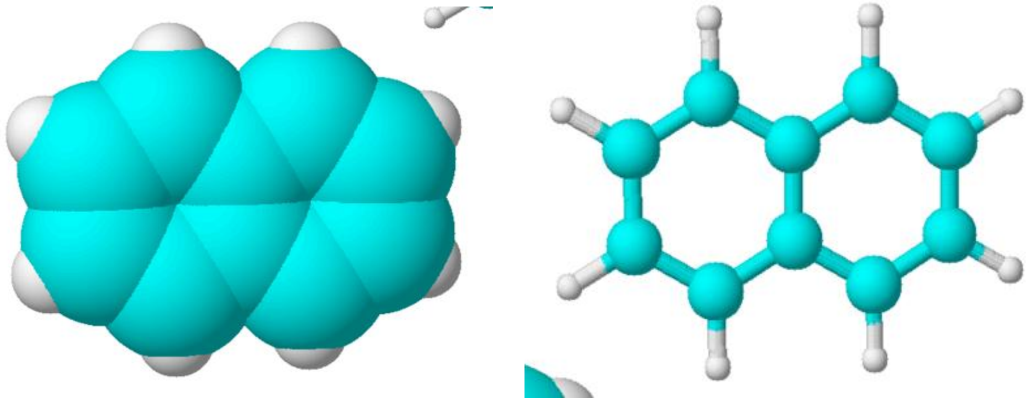


Figure 15.26 The simplest polycyclic aromatic molecule, $C_{10}H_8$, represented as (a) a space-filling model, and (b) a ball-and-stick model.

15.9 Where Next?

In this Chapter, the wide variety of compounds of carbon and hydrogen has been discussed. In the final chapter, Chapter 16, it will be shown that there is an even wider variety of organic compounds if other elements – particularly oxygen – are incorporated in the molecular structure.