# 6.2: Compounds of Carbon and Hydrogen - Hydrocarbons

The tremendous variety and diversity of organic chemistry is due to the ability of carbon atoms to bond with each other in a variety of straight chains, branched chains, and rings and of adjacent carbon atoms to be joined by single, double, or triple bonds. This bonding ability can be illustrated with the simplest class of organic chemicals, the **hydrocarbons** consisting only of hydrogen and carbon. Figure 6.1 shows some hydrocarbons in various configurations. Hydrocarbons are the major ingredients of petroleum and are pumped from the ground as crude oil or extracted as natural gas. They have two major uses. The first of these is combustion as a source of fuel. The most abundant hydrocarbon in natural gas, methane, $CH_4$, is burned in home furnaces, electrical power plants, and even in vehicle engines,

$$\mathrm{CH_4 + 2\,O_2 \rightarrow CO_2 + 2\,H_2O + heat energy} \tag{6.2.1}$$

to provide energy. The second major use of hydrocarbons is as a raw material for making rubber, plastics, polymers, and many other kinds of materials. Given the value of hydrocarbons as a material, it is unfortunate that so much of hydrocarbon production is simply burned to provide energy, which could be generated by other means.

There are several major class of hydrocarbons, all consisting of only hydrogen and carbon. **Alkanes** have only single bonds between carbon atoms. Cyclohexane, *n*-heptane, and 3-ethyl-2,5-dimethylhexane in Figure 6.1 are alkanes; the cyclohexane is a cyclic hydrocarbon. **Alkenes**, such as propene shown in Figure 6.1, have at least one double bond consisting of 4 shared electrons between two of the carbon atoms in the molecule. **Alkynes** have at least one triple bond between carbon atoms in the molecule as shown for acetylene in Figure 6.1. Acetylene is an important fuel for welding and cutting torches; otherwise, the alkynes are of relatively little importance and will not be addressed farther. A fourth class of hydrocarbon consists of **aromatic** compounds which have rings of carbon atoms with special bonding properties as discussed later in this chapter

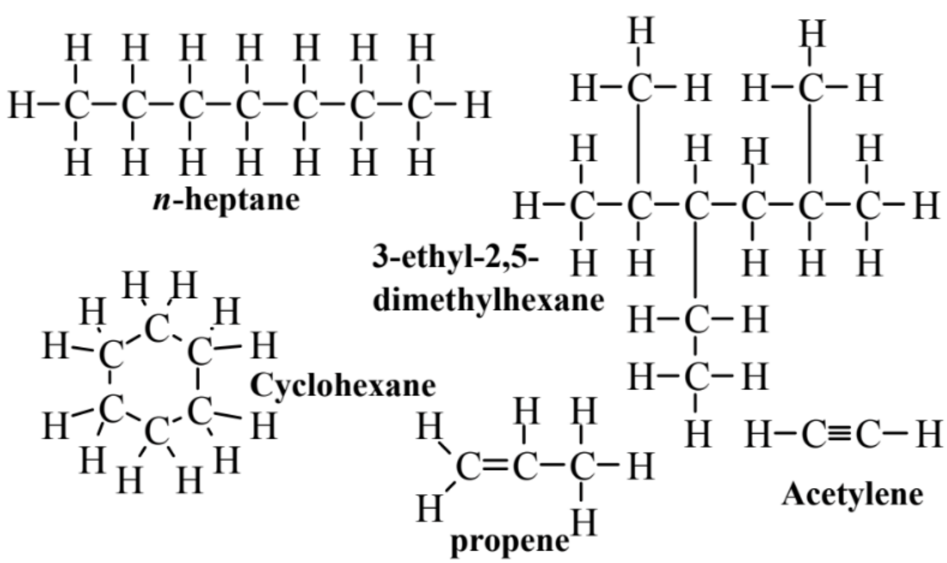



Figure 6.1. Some typical hydrocarbons. These formulas illustrate the bonding diversity of carbon which gives rise to an enormous variety of hydrocarbons and other organic compounds.

## Alkanes

The molecular formulas of non-cyclic alkanes are CnH2n+2. By counting the numbers of carbon and hydrogen atoms in the molecules of alkanes shown in Figure 6.1, it is seen that the molecular formula of *n*-heptane is $C_7H_6$ and that of 3-ethyl-2,5-dimethylhexane is $C_{10}H_{22}$, both of which fit the general formula given above. The general formula of cyclic alkanes is $C_nH_{2n}$; that of cyclohexane, the most common cyclic alkane, is $C_6H_{12}$. These formulas are **molecular formulas**, which give the number of carbon and hydrogen atoms in each molecule, but do not tell anything about the structure of the molecule. The formulas given in Figure 6.1 are **structural formulas** which show how the molecule is assembled. The structure of *n*-heptane is that of a straight chain of carbon atoms; each carbon atom in the middle of the chain is bound to 2 H atoms and the 2 carbon atoms at the ends of the chain are each bound to 3 H atoms. The prefix *hep* in the name denotes 7 carbon atoms and the*n*-indicates that the compound consists of a single straight chain. This compound can be represented by a **condensed structural formula** as $CH_3(CH_2)_5CH_3$

representing 7 carbon atoms in a straight chain. In addition to methane mentioned previously, the lower alkanes include the following:

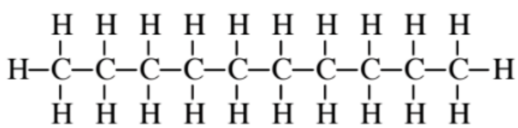
Ethane: $CH_3CH_3$ Propane: $CH_3CH_2CH_3$ Butane: $CH_3(CH_2)_2CH_3$ *n*-Pentane: $CH_3(CH_2)3CH_3$

For alkanes with 5 or more carbon atoms, the prefix (*pen* for 5,*hex* for 6,*hept* for 7,*oct* for 8,*non* for 9) shows the total number of carbon atoms in the compound and *n*-may be used to denote a straight-chain alkane. Condensed structural formulas may be used to represent branched chain alkanes as well. The condensed structural formula of 3-ethyl-2,5-dimethylhexane is

$$CH_3CH(CH_3)CH(C_2H_5)CH_2CH(CH_3)CH_3$$

In this formula, the C atoms and their attached H atoms that are not in parentheses show carbons that are part of the main hydrocarbon chain. The ($CH_3$) after the second C in the chain shows a methyl group attached to it, the ($C_2H_5$) after the third carbon atom in the chain shows an ethyl group attached to it, and the ($CH_3$) after the fifth carbon atom in the chain shows a methyl group attached to it.

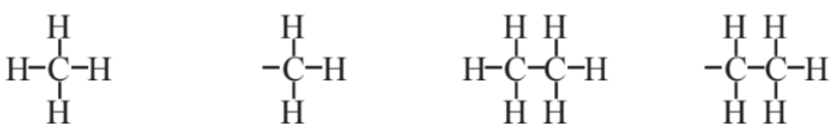
Compounds that have the same molecular formulas but different structural formulas are **structural isomers**. For example, the straight-chain alkane with the molecular formula $C_{10}H_{22}$ is *n*-decane



***n*-decane**

which is a structural isomer of 3-ethyl-2,5-dimethylhexane.

The names of organic compounds are commonly based upon the structure of the hydrocarbon from which they are derived using the longest continuous chain of carbon atoms in the compound as the basis for the name. For example, the longest continuous chain of carbon atoms in 3-ethyl-2,5-dimethylhexane shown in Figure 6.1 is 6 carbon atoms, so the name is based upon *hex*ane. The names of the chain branches are also based upon the alkanes from which they are derived. As shown below,



**Methane ($CH_4$) Methyl group ($CH_3$) Ethane ($C_2H_6$) Ethyl group ($C_2H_5$)**

the two shortest-chain alkanes are methane with 1 carbon atom and ethane with 2 carbon atoms. Removal of 1 of the H atoms from methane gives the **methyl** group and removal of 1 of the H atoms from ethane gives the **ethyl** group. These terms are used in the name 3-ethyl-2,5-dimethylhexane to show groups attached to the basic hexane chain. The carbon atoms in this chain are numbered sequentially from left to right. An ethyl group is attached to the 3rd carbon atom, yielding the "3-ethyl" part of the name, and methyl groups are attached to the 2nd and 5th carbon atoms, which gives the "2,5-dimethyl" part of the name.

The names discussed above are **systematic names**, which are based upon the actual structural formulas of the molecules. In addition, there are **common names** of organic compounds that do not indicate the structural formulas. Naming organic compounds is a complex topic, and no attempt is made here to teach it to the reader. However, from the names of compounds given in this and later chapters, some appreciation of the rationale for organic compound names should be obtained.

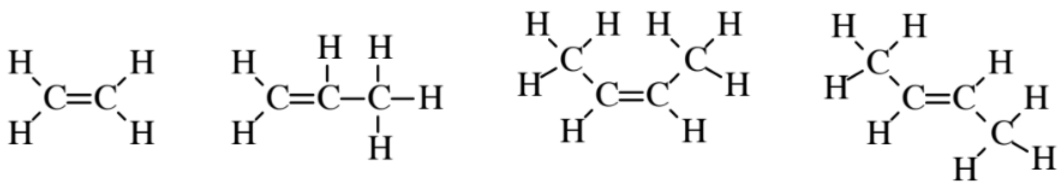
Other than burning them for energy, the major kind of reaction with alkanes consists of **substitution reactions** such as,

$$C_2H_6 + 2\,Cl_2 \rightarrow C_2H_4Cl_2 + 2\,HCl \tag{6.2.2}$$

in which one or more H atoms are displaced by another kind of atom. This is normally the first step in converting alkanes to compounds containing elements other than carbon or hydrogen for use in synthesizing a wide variety of organic compounds.

**Alkenes**

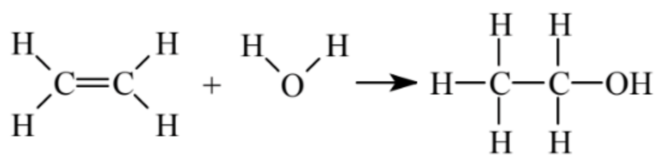
Four common alkenes are shown in Figure 6.2. Alkenes have at least one C=C double bond per molecule and may have more. The first of the alkenes in Figure 6.2, ethylene, is a very widely produced hydrocarbon used to synthesize polyethylene plastic and other organic compounds. About 25 billion kilograms (kg) of ethylene are processed in the U.S. each year. About 14.5 billion kg of propylene are used in the U.S. each year to produce polypropylene plastic and other chemicals. The two 2-butene compounds illustrate an important aspect of alkenes, the possibility of ***cis-trans*** isomerism. Whereas carbon atoms and the groups substituted onto them joined by single bonds can freely rotate relative to each other as though they were joined by a single shaft, carbon atoms connected by a double bond behave as though they were attached by two parallel shafts and are not free to rotate. So, *cis*-2-butene in which the two end methyl (-CH3) groups are on the same side of the molecule is a different compound from *trans*-2-butene in which they are on opposite sides. These two compounds are *cis*-*trans* isomers



**Ethylene** **Propylene (propene)** ***Cis*-2-butene** ***Trans*-2-butene**

Figure 6.2. Examples of alkene hydrocarbons

Alkenes are chemically much more active than alkanes. This is because the double bond is **unsaturated** and has electrons available to form additional bonds with other atoms. This leads to **addition reactions** in which a molecule is added across a double bond. For example, the addition of $H_2O$ to ethylene

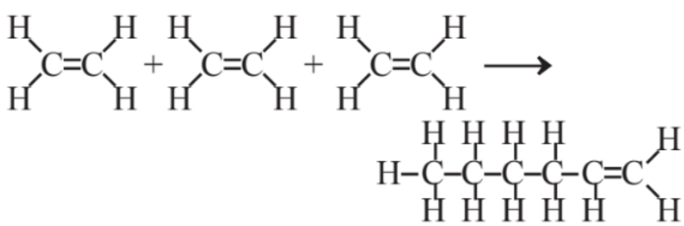


(6.2.3)

**Ethylene** **Water** **Ethanol**

yields ethanol, the same kind of alcohol that is in alcoholic beverages. In addition to adding immensely to the chemical versatility of alkenes, addition reactions make them quite reactive in the atmosphere during the formation of photochemical smog. The presence of double bonds also adds to the biochemical and toxicological activity of compounds in organisms

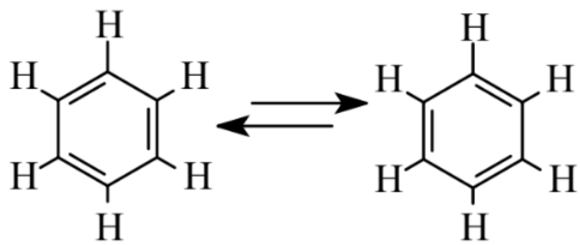
Because of their double bonds, alkenes can undergo **polymerization** reactions in which large numbers of individual molecules add to each other to produce big molecules called **polymers** (see Section 6.5). For example, 3 ethylene molecules can add together as follows:



a process that can continue, forming longer and longer chains and resulting in the formation of huge molecules molecules of polyethylene

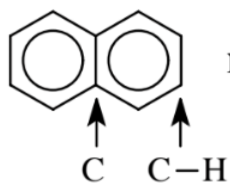
**Aromatic Hydrocarbons**

A special class of hydrocarbons consists of rings of carbon atoms, almost always containing 6C atoms, which can be viewed as having alternating single and double bonds as shown below:



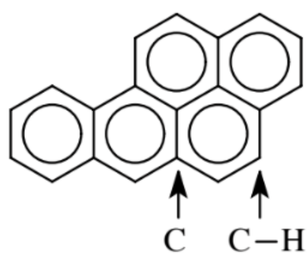

These structures show the simplest aromatic hydrocarbon, benzene, C6H6. Although the benzene molecule is represented with 3 double bonds, chemically it differs greatly from alkenes, for example undergoing substitution reactions rather than addition reactions. The properties of aromatic compounds are special properties called **aromaticity**. The two structures shown above are equivalent **resonance** structures, which can be viewed as having atoms that stay in the same places, but in which the bonds joining the atoms can shift positions with the movement of electrons composing the bonds. Since benzene has different chemical properties from those implied by either of the above structures, it is commonly represented as a hexagon with a circle in the middle:

Many aromatic hydrocarbons have two or more rings. The simplest of these is naphthalene,




**Naphthalene, $C_{10}H_8$**

a two-ringed compound in which two benzene rings share the carbon atoms at which they are joined; these two carbon atoms do not have any H attached, each of the other 8 C atoms in the compound has 1 H attached. Aromatic hydrocarbons with multiple rings, called **polycyclic aromatic hydrocarbons**, PAH, are common and are often produced as byproducts of combustion. One of the most studied of these is benzo(a)pyrene,




**Benzo(a)pyrene, $C_{20}H_{12}$**

found in tobacco smoke, diesel exhaust, and charbroiled meat. This compound is toxicologically significant because it is partially oxidized by enzymes in the body to produce a cancer-causing metabolite.

The presence of hydrocarbon groups and of elements other than carbon and hydrogen bonded to an aromatic hydrocarbon ring gives a variety of **aromatic compounds**. Three examples of common aromatic compounds are given below. Toluene is widely used for chemical synthesis and as a solvent. The practice of green chemistry now calls for substituting toluene for benzene wherever possible because benzene is suspected of causing leukemia, whereas the body is capableof metabolizing toluene to harmless metabolites (see Chapter 7). About 850 million kg of aniline are made in the U.S. each year as an intermediate in the synthesis of dyes and other organic chemicals. Phenol is a relatively toxic oxygen-containing aromatic compound which, despite its toxicity to humans, was the first antiseptic used in the 1800s.


$CH_3$
Toluene
$NH_2$
Aniline
OH
Phenol