# 12.3: The Structure of Organic Molecules - Alkanes and Their Isomers

**Learning Objectives**

- To identify simple alkanes as straight-chain or branched-chain.
- Describe and recognize structural and functional group isomers.

As you just learned, there is a wide variety of organic compounds containing different functional groups. However, all organic compounds are hydrocarbons, they contain hydrogen and carbon. The general rule for hydrocarbons is that any carbon must be bonded to at least one other carbon atom, except in the case of methane which only contains one carbon. The bonded carbons form the *backbone* of the molecule to which the hydrogen atoms (or other functional groups) are attached.

Hydrocarbons with only carbon-to-carbon single bonds (C–C) are called **alkanes** (or saturated hydrocarbons). *Saturated*, in this case, means that each carbon atom is bonded to four other atoms (hydrogen or carbon)—the most possible; there are no double or triple bonds in these molecules.

> Saturated fats and oils are organic molecules that do not have carbon-to-carbon double bonds (C=C).

The three simplest alkanes—methane ($CH_4$), ethane ($C_2H_6$), and propane ($C_3H_8$) shown in Figure 12.3.1, are the beginning of a series of compounds in which any two members in a sequence differ by one carbon atom and two hydrogen atoms—namely, a $CH_2$ unit (called methylene). Alkanes follow the general formula: $C_nH_{2n+2}$. Using this formula, we can write a molecular formula for any alkane with a given number of carbon atoms. For example, an alkane with eight carbon atoms has the molecular formula $C_8H_{(2 \times 8) + 2} = C_8H_{18}$.

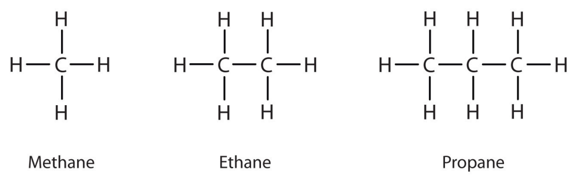
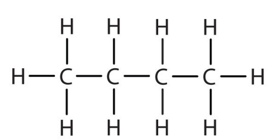



Figure 12.3.1: The Three Simplest Alkanes

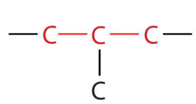
## Isomers

Alkanes that contain one continuous chain of linked carbons are called **straight-chain** alkanes. As the number of carbons in a chain increases beyond three, the arrangement of atoms can expand to include **branched-chain** alkanes. In a branched chain, one or more hydrogen atoms along the chain is replaced by a carbon atom (or a separate chain of carbon atoms). It is important to note that while the structural arrangement of these chains are different, continuous versus branched, they both still follow the same general formula for alkanes as introduced above, $C_nH_{2n+2}$. In fact, alkane chains that have the same molecular formula (same number of carbon and hydrogen), but a different arrangement of atoms, are called **isomers**. Let's look at an example below:

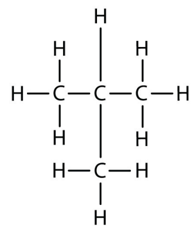
The structure of butane ($C_4H_{10}$) is written by stringing four carbon atoms in a row, and then adding enough hydrogen atoms to give each carbon atom four bonds:



Butane is a straight-chain alkane, but there is another way to put 4 carbon atoms and 10 hydrogen atoms together. Place 3 of the carbon atoms in a row and then *branch* the fourth carbon off the middle carbon atom:



Now we add enough hydrogen atoms to give each carbon four bonds:



The result is the isomer 2-methylpropane (also called isobutane), which is a branched-chain alkane with the same formula as butane, ($C_4H_{10}$). However, it is a *different* molecule with a *different* name and *different* chemical properties. A side-by-side comparison of these two molecules is shown in the below figure.

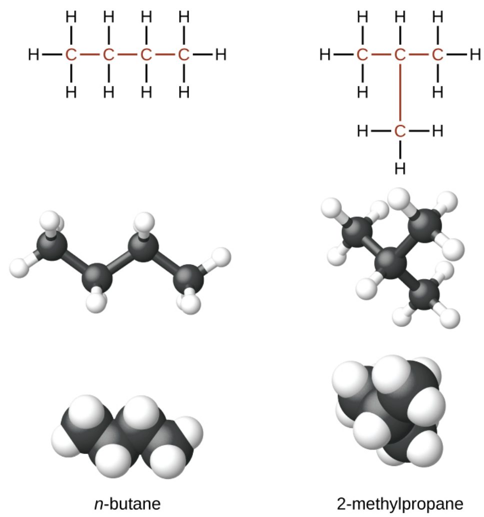



Figure 12.3.1: n-butane and 2-methylpropane. The compounds *n*-butane and 2-methylpropane are structural isomers, meaning they have the same molecular formula, $C_4H_{10}$, but different spatial arrangements of the atoms in their molecules. We use the term *normal*, or the prefix *n*, to refer to a chain of carbon atoms without branching.

The four-carbon straight chain butane may be drawn with different bends or kinks in the backbone (Figure 12.3.2) because the groups can rotate freely about the C–C bonds. This rotation or bending of the carbon chain does *not* change the identity of the compound; all of the following structures represent the *same* compound, butane, with different bends in the chain:

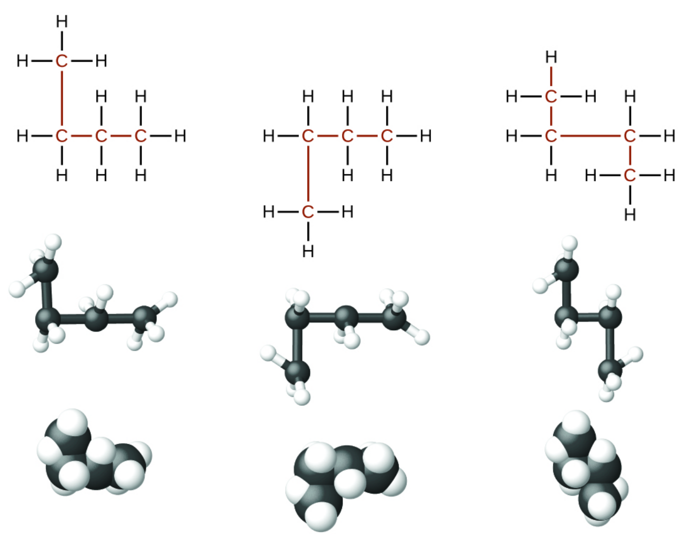
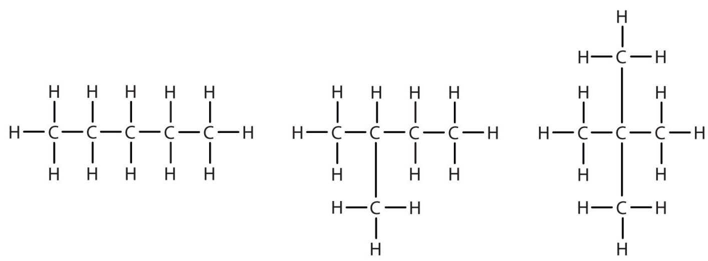


Figure 12.3.2: These three representations of the structure of n-butane are not isomers because they all contain the same arrangement of atoms and bonds.

When identifying isomers, it is useful to trace the carbon backbone with your finger or a pencil and count carbons until you need to lift your hand or pencil to get the another carbon. Try this with each of the above arrangements of four carbons, then do the same with 2-methylpropane. Butane has a continuous chain of four carbons no matter how the bonds are rotated – you can connect the carbons in a line without lifting your finger from the page. How many continuous carbons are in the 2-methylpropane backbone? You should be able to count a continuous chain of three carbon atoms only, with the fourth carbon attached as a branch, (compare the two structures in Figure 12.3.1). In a later chapter, you will learn how to systematically name compounds by counting the number of carbons in the longest continuous chain and identifying any functional groups present.

Adding one more carbon to the butane chain gives pentane, which has the formula, $C_5H_{12}$. Pentane and its two branched-chain isomers are shown below. The compound at the far left is pentane because it has all five carbon atoms in a continuous chain. The compound in the middle is isopentane; like isobutane, it has a one $CH_3$ branch off the second carbon atom of the continuous chain. The compound at the far right, discovered after the other two, was named neopentane (from the Greek *neos*, meaning "new"). Although all three have the same molecular formula, they have different properties, including boiling points: pentane, 36.1°C; isopentane, 27.7°C; and neopentane, 9.5°C. The names isopentane and neopentane are common names for these molecules. As mentioned above, we will learn the systematic rules for naming compounds in later chapters.



Pentane Isopentane Neopentane

> A continuous (unbranched) chain of carbon atoms is often called a *straight chain* even though the tetrahedral arrangement about each carbon gives it a zigzag shape. Straight-chain alkanes are sometimes called *normal alkanes*, and their names are given the prefix *n*-. For example, butane is called *n*-butane. We will not use that prefix here because it is not a part of the system established by the International Union of Pure and Applied Chemistry.