12.4: Branched Alkanes

The ball-and-stick models you have seen thus far in this text use a rendering tool for viewing molecules online called JSmol. JSmol was designed to replicate molecular model kits (see Figure 12.4.1) that have long been used in chemistry classes to represent three-dimensional structures of molecules.

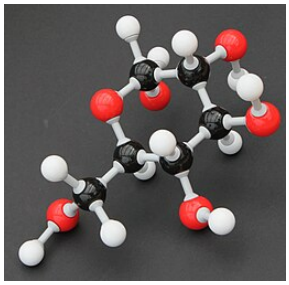
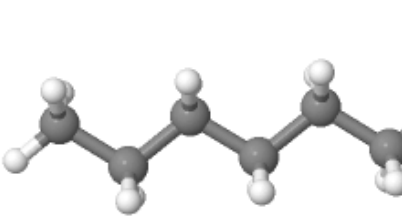
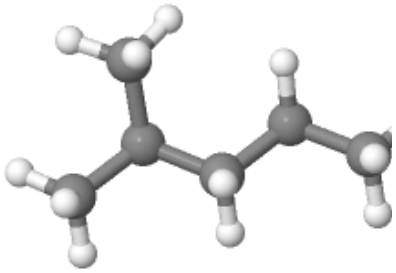


Figure 12.4.1: A molecular model kit used to build three-dimensional molecular models. [Sonia (left) and Bin im Garten (right), via Wikimedia Commons]

A common hands-on activity is to provide students with molecular model kits to build models that have a specified chemical formula and to compare the models. There are millions of examples that may be selected for comparison, but if that formula was C_6H_{14}, students would soon notice that there are five different ways to build a molecule of C_6H_{14}. Substances that have the same molecular formula, but a different arrangement of atoms are called **isomers**. The five isomers of C_6H_{14} are shown in Figure 12.4.2:





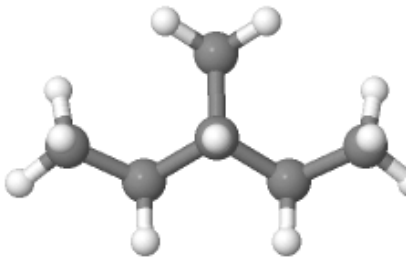


Figure 12.4.2: The five isomers of C_6H_{14}.

Molecules rendered in JSmol may be rotated in all directions to examine molecules in different orientations. Simply "grab" onto the molecule and drag in the desired direction(s) as shown in Figure 12.4.3. Try rotating the molecules in Figure 12.4.2 above to make all 14 hydrogen atoms visible in each isomer. *Go ahead...try it!*

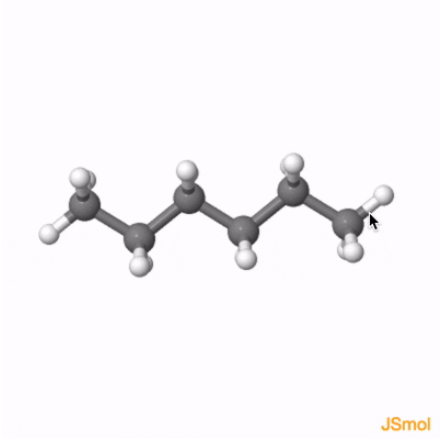


Figure 12.4.3: Rotating a hexane molecule rendered with JSmol.

IUPAC Nomenclature

While molecules are written or drawn in two dimensions, it is important to remember that molecules are three-dimensional. Since isomers of each other are unique, they have different chemical and physical properties. The differences are sometimes small and at other times, quite significant. To distinguish isomers from one another, it is important that they be assigned a unique name. The International Union of Pure and Applied Chemistry (IUPAC) has devised a system of nomenclature that begins with the names of the alkanes and can be adjusted from there to account for more complicated structures.

Success with organic nomenclature begins with the ability to count carbon atoms. Similar to how Greek prefixes were used to designate a specific number of atoms in binary molecular compounds, IUPAC nomenclature uses prefixes based on the alkanes to designate a specific number of carbon atoms. Notice that Greek prefixes are used for specifying five or more carbon atoms.

Table 12.4.1: IUPAC Prefixes Used to Specify the Number of Carbon Atoms in Organic Compounds

Number of Carbon Atoms	IUPAC Prefix	Number of Carbon Atoms	IUPAC Prefix

Number of Carbon Atoms	IUPAC Prefix	Number of Carbon Atoms	IUPAC Prefix
1	meth-	6	hex-
2	eth-	7	hept-
3	prop-	8	oct-
4	but-	9	non-
5	pent-	10	dec-

Branched Alkanes

The isomers of C_6H_{14} shown in Figure 12.4.2 above are shown again in Table 12.4.2 below along with their condensed structural formulas, line formulas, and IUPAC names. While we already learned how to name hexane and other straight-chained alkanes in the previous section, the remaining isomers of C_6H_{14} are branched. How are the names for these branched molecules determined? Here are some basic guidelines:

☞ IUPAC Nomenclature of Branched Alkanes

1. Identify and name the **parent chain**.
   - The **parent chain** is the longest consecutive chain of carbon atoms in the molecule.

2. Identify and name all branches off the parent chain as **alkyl groups**.
   - An **alkyl group** is an alkane that has had one H atom removed.
   - If the H atom is removed from the end carbon of a straight-chain alkane, the alkyl group is named by changing the *–ane* suffix of the alkane to *–yl*.
   - The name(s) of the alkyl group(s) precedes the name of the parent chain.
   - Common alkyl groups:

methyl	CH_3-
ethyl	CH_3CH_2-
propyl	$CH_3CH_2CH_2-$
isopropyl	$CH_3\underset{\vert}{C}HCH_3$
butyl	$CH_3CH_2CH_2CH_2-$

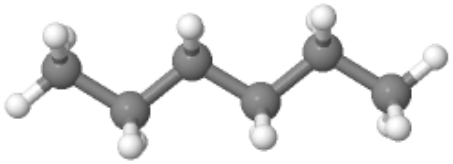
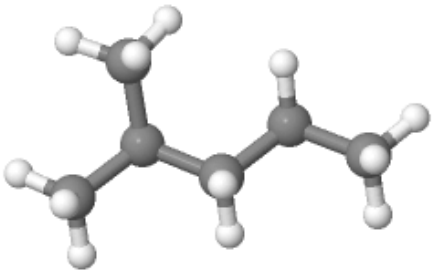
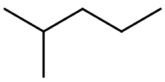
3. Locate and assign a number to the position of each branch off the parent chain.
   - For a single branch off the parent chain:
     - Count in the direction that gives the lowest number.
     - Place the number in front of the name of the alkyl group, separating the number and name with a hyphen (Example: 3-methyl).
   - For multiple branches off the parent chain:
     - Count in the direction that gives the lowest number for any branch off the parent chain.
     - For branches of the same type:
       - Indicate the number of that type by using the Greek prefixes *di–*, *tri–*, *tetra–*, etc. in front of the name of the alkyl group.
       - Write the number of the position of each branch in ascending order, separating the numbers by commas.
       - Example: 2,3,3-trimethylheptane
     - For branches of different types:
       - The alkyl groups are named in alphabetical order, with a number indicating the position of each alkyl group off the parent chain.

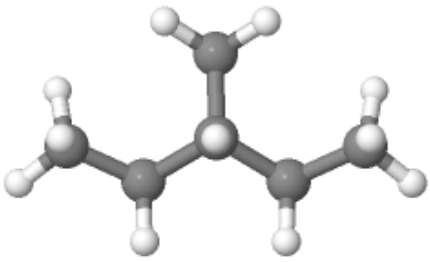
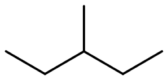
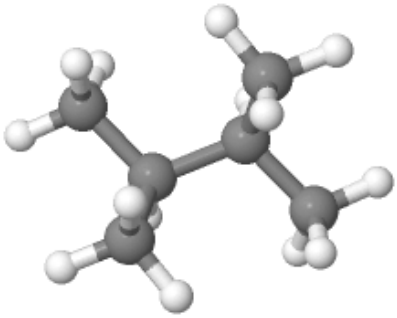
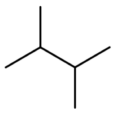
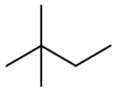
- Example: 3-ethyl-2-methylhexane

4. Additional Notes:

- The name of an alkane has no spaces.
- Numbers are separated by commas. Numbers and letters are separated by hyphens.
- Whether branched or unbranched, alkanes always have a general formula of C_nH_{2n+2}.

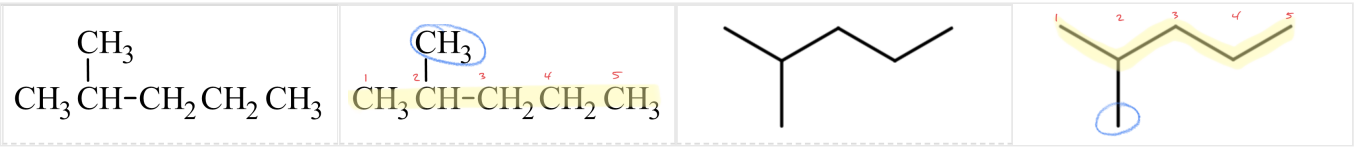
Table 12.4.2: The Five Isomers of C_6H_{14}.

Three-Dimensional Structure	Condensed Structural Formula	Line Formula	IUPAC Name
 JSmol	$CH_2\,CH_3$		hexane
 JSmol	$_2\,CH_3$		2-methylpentane

Three-Dimensional Structure	Condensed Structural Formula	Line Formula	IUPAC Name
 JSmol	$_2CH_3$		3-methylpentane
 JSmol	CH_3		2,3-dimethylbutane
unrecognized file format for file https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/cid/6403/SDF?recor error JSmol	CH_3		2,2-dimethylbutane

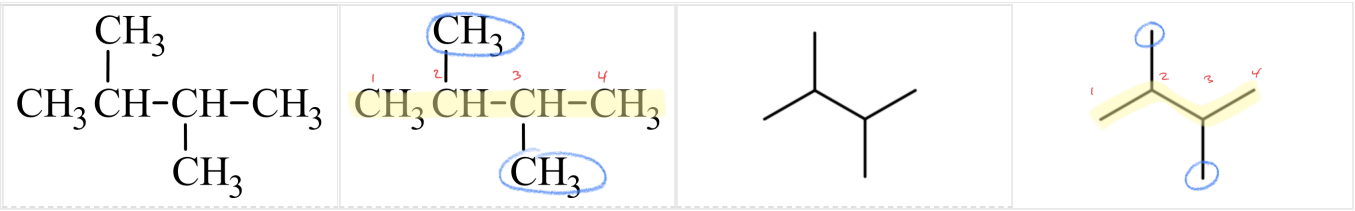
Let's look at how the name 2-methylpentane is derived. Following the guidelines for the IUPAC Nomenclature of Branched Alkanes listed above:

1. The parent chain has five carbon atoms, or *pentane*.
2. There is a one-carbon alkyl group that is branched off of the parent chain. If a one-carbon alkane is called methane, then a one-carbon alkyl group is called a *methyl group*. There are no spaces in the name, so *methyl* is written in front of *pentane*, giving us *methylpentane*.
3. The *methyl group* is branched off of the second carbon atom in the parent chain, so *2* is written in front of *methylpentane*. Letters and numbers are separated with a hyphen, making it *2-methylpentane*.



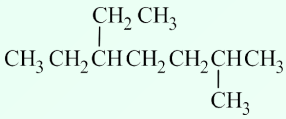
Next, lets look at how the name 2,3-dimethylbutane is derived. Following the guidelines for the IUPAC Nomenclature of Branched Alkanes listed above:

1. The parent chain has four carbon atoms, or *butane*.
2. There are two *methyl* groups branched off of the parent chain, which means that *dimethyl* is written in front of *butane*, making it *dimethylbutane*.
3. One *methyl group* is branched off the second carbon atom of the parent chain and one is branched off the third carbon atom, so *2,3-* is written in front of *dimethylbutane*, making it *2,3-dimethylbutane*.

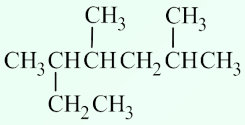


✅ **Example 12.4.1**

Write the IUPAC name for each molecule.

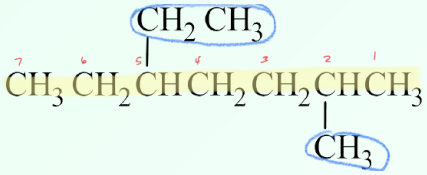


A.



B.

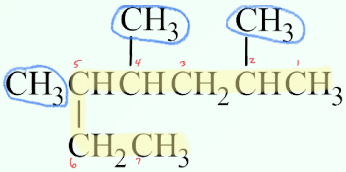
Solution



A.

1. The parent chain has seven carbon atoms, yielding a name of *heptane*.
2. There is one *ethyl* group and one *methyl* group branched off of the parent chain.
3. The parent chain is numbered from *right to left*, since this gives the lowest number for any branch off of the parent chain.

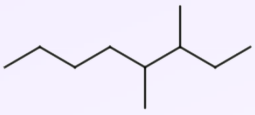
4. The *methyl* group is branched off the 2nd carbon on the parent chain (making it *2-methyl*) and the *ethyl* group is branched off the 5th carbon atom on the parent chain (making it *5-ethyl*).
5. Alphabetically, *ethyl* comes before *methyl*, so *5-ethyl* comes first in the name, making it *5-ethyl-2-methylheptane*.

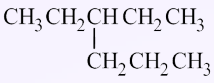
B. 

1. The parent chain has seven carbon atoms, which is longer than the six consecutive carbon atoms obtained by tracing straight across the molecule. Therefore, the parent chain is named *heptane*.
2. There are three *methyl* groups branched off of the parent chain, which means that *trimethyl* is written in front of *heptane*, yielding *trimethylheptane*.
3. The parent chain is numbered from *right to left*, since this gives the lowest number for any branch off of the parent chain.
4. The *methyl groups* are branched off the second, fourth, and fifth carbon atoms of the parent chain, so *2,4,5-* is written in front of *trimethylheptane*, making it *2,4,5-trimethylheptane*.

Exercise 12.4.1

Write the IUPAC name for each molecule.

A. 

B. 

Answer A

3,4-dimethyloctane

Answer B

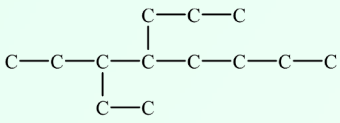
3-ethylhexane

Example 12.4.2

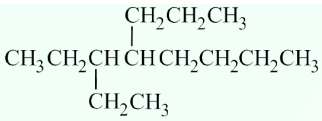
Write the condensed structural formula and line formula for each.

A. 3-ethyl-4-propyloctane
B. 3,3-dimethylhexane

Solution

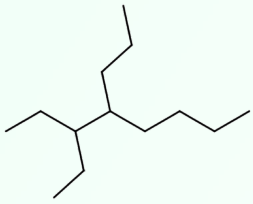
A. 

It's often the easiest to begin by drawing out the skeleton structure. The name *octane* indicates the parent chain has eight carbon atoms. An *ethyl* group has two carbon atoms and is branched off the 3rd carbon atom on the parent chain. A *propyl* group has three carbon atoms and is branched off the 4th carbon atom on the parent chain.



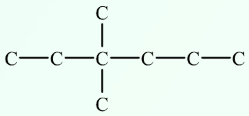
From here, fill in the H atoms. Remember that hydrogen can only make one bond, while carbon makes four. If a carbon atom is bonded to one other atom by a single bond, it can hold three hydrogen atoms. If a carbon atom makes three bonds to other atoms, it can only hold one hydrogen atom.

Once all of the hydrogen atoms have been added, you can check to see if the structure conforms to the general formula for alkanes, C_nH_{2n+2}. Since there are 13 carbon atoms, there should be 2(13) + 2 = 28 hydrogen atoms. Summing together all of the hydrogen atoms in the condensed structural formula shows the formula is indeed $C_{13}H_{28}$.

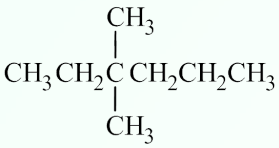


The line formula is shown above. The parent chain shows a total of eight ends or bends. There are two carbon atoms branched off the third carbon of the parent chain. There are three carbon atoms branched off the fourth carbon of the parent chain.

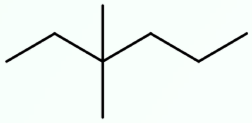
B.



Begin by drawing the skeleton structure. The name *hexane* indicates the parent chain has six carbon atoms. A *methyl* group has one carbon atom. The prefix *di–* indicates there are two *methyl* groups. Both *methyl* groups are branched off the 3rd carbon atom on the parent chain.



From here, fill in the H atoms. Each hydrogen makes one bond, while carbon makes four. Once all of the hydrogen atoms have been added, you can check to see if the structure conforms to the general formula for alkanes, C_nH_{2n+2}. Since there are 8 carbon atoms, there should be 2(8) + 2 = 18 hydrogen atoms. Summing together all of the hydrogen atoms in the condensed structural formula shows the formula is indeed C_8H_{18}.

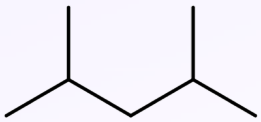


The line formula is shown above. The parent chain shows a total of six ends or bends. There are two one-carbon atom branches off the third carbon of the parent chain.

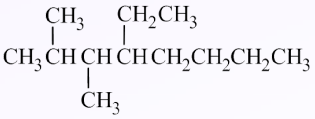
Exercise 12.4.2

A. Draw the line structure of 2,4-dimethylpentane.
B. Write the condensed structural formula of 4-ethyl-2,3-dimethyloctane.

Answer A



Answer B



Summary

- A structural isomer is one of multiple molecules that have the same molecular formula, but different structural formulas.
- Nomenclature rules for branched hydrocarbons are given.