4.4B Naming an Acyclic Alkane

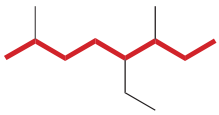
Four steps are needed to name an alkane.

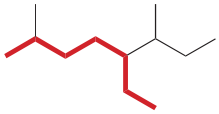
How To Name an Alkane Using the IUPAC System

Step [1] Find the parent carbon chain and add the suffix.

- Find the longest continuous carbon chain, and name the molecule by using the parent name for that number of carbons, given in Table 4.1. To the name of the parent, add the suffix ***-ane*** for an alkane. Each functional group has its own characteristic suffix.

Correct **Incorrect**

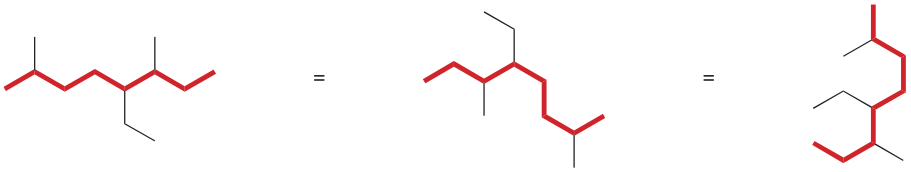




8 C's in the longest chain
8 C's ----→ **octane**

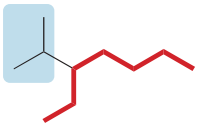
7 C's in the longest chain

- Finding the longest chain is a matter of trial and error. Place your pencil on one end of the chain, go to the other end without picking it up, and count carbons. Repeat this procedure until you have found the chain with the largest number of carbons.
- It does not matter if the chain is *straight* or has *bends*. All of the following representations are equivalent, and each longest chain has eight carbons.



- If there are two chains of equal length, pick the chain with more substituents. In the following example, two different chains in the same alkane contain 7 C's, but the compound on the left has two alkyl groups attached to its long chain, whereas the compound to the right has only one.

Correct **Incorrect**



7 atoms in the longest chain
2 substituents

more substituents

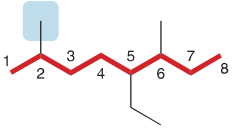
7 atoms in the longest chain
only 1 substituent

fewer substituents

Step [2] Number the atoms in the carbon chain.

- Number the longest chain to give the *first* substituent the lower number.

Correct **Incorrect**



first substituent at C2

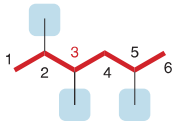
first substituent at C3

—*Continued*

How To, continued . . .

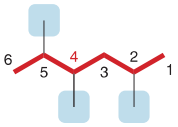
- If the first substituent is the same distance from both ends, number the chain to give the *second* substituent the lower number. Always look for the first point of difference in numbering from each end of the longest chain.

Correct



CH_3 groups at C2, C3, and C5
The second CH_3 group has the lower number (C3).

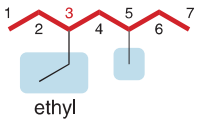
Incorrect



CH_3 groups at C2, C4, and C5
The second CH_3 group has the higher number (C4).

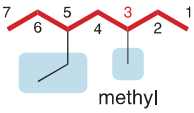
- When numbering a carbon chain results in the same numbers from either end of the chain, assign the lower number *alphabetically* to the first substituent.

Correct



- **e**thyl at **C3**
- **m**ethyl at **C5**

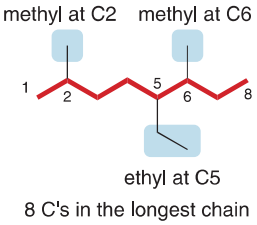
Incorrect



- **m**ethyl at **C3**
- **e**thyl at **C5**

Earlier letter ⟶ lower number

Step [3] Name and number the substituents.

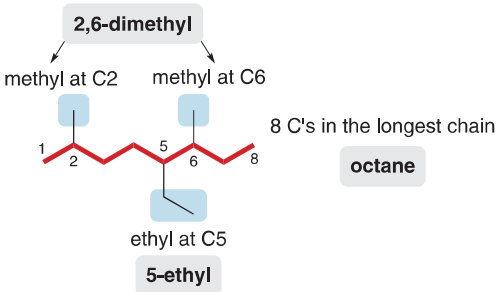


- Name the substituents as alkyl groups, and use the numbers from Step 2 to designate their location.
- Every carbon belongs to *either* the longest chain or a substituent, but *not both.*
- Each substituent needs its *own* number.
- If two or more identical substituents are bonded to the longest chain, use prefixes to indicate how many: **di-** for two groups, **tri-** for three groups, **tetra-** for four groups, and so forth. This molecule has two methyl substituents, so its name contains the prefix di- before the word methyl → *di*methyl.

Step [4] Combine substituent names and numbers + parent + suffix.

- Precede the name of the parent by the names of the substituents.
- Alphabetize the names of the substituents, ignoring all prefixes except *iso,* as in isopropyl and isobutyl.
- Precede the name of each substituent by the number that indicates its location. There must be **one number for each substituent.**
- Separate numbers by commas and separate numbers from letters by hyphens. The name of an alkane is a single word, with no spaces after hyphens or commas.

[1] Identify all the pieces of a compound, using Steps 1–3.



[2] Then, put the pieces of the name together.

substituent names and numbers + parent + suffix

5-ethyl-2,6-dimethyl + **oct** + **ane**

Alphabetize: **e** for **ethyl,** then **m** for **methyl**

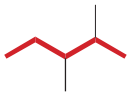
8 C's

an **alkane**

Answer: 5-ethyl-2,6-dimethyloctane

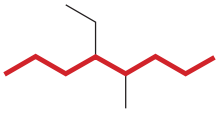
Several additional examples of alkane nomenclature are given in Figure 4.1.

Figure 4.1
Examples of alkane nomenclature



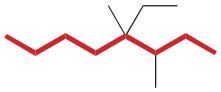
2,3-dimethylpentane

Number to give the 1st methyl group the lower number.



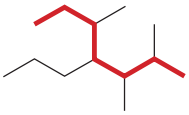
4-ethyl-5-methyloctane

Assign the lower number to the 1st substituent alphabetically: the **e** of **e**thyl before the **m** of **m**ethyl.



4-ethyl-3,4-dimethyloctane

Alphabetize the **e** of **e**thyl before the **m** of **m**ethyl.

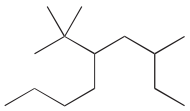


2,3,5-trimethyl-4-propylheptane

Pick the long chain with more substituents.

- The carbon atoms of each long chain are drawn in **red**.

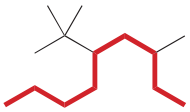
Sample Problem 4.1 Give the IUPAC name for the following compound.



Solution

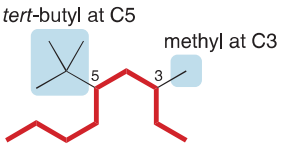
To help identify which carbons belong to the longest chain and which are substituents, box in or highlight the atoms of the long chain. Every other carbon atom then becomes a substituent that needs its own name as an alkyl group.

Step 1: Name the parent.

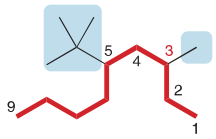


9 C's in the longest chain
nonane

Step 3: Name and number the substituents.



Step 2: Number the chain.



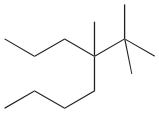
first substituent at C3

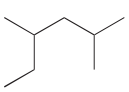
Step 4: Combine the parts.

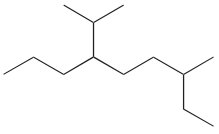
- Alphabetize: the **b** of **butyl** before the **m** of **methyl**

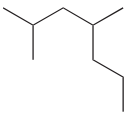
Answer: 5-*tert*-butyl-3-methylnonane

Problem 4.7 Give the IUPAC name for each compound.

a. 

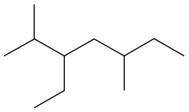
b. 

c. 

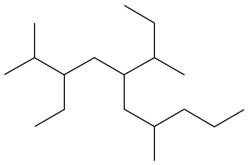
d. 

Problem 4.8 Give the IUPAC name for each compound.

a. $(CH_3)_3CCH_2CH(CH_2CH_3)_2$

b. 

c. $CH_3(CH_2)_3CH(CH_2CH_2CH_3)CH(CH_3)_2$

d. 

You must also know how to derive a structure from a given name. Sample Problem 4.2 illustrates a stepwise method.

Sample Problem 4.2 Give the structure corresponding to the following IUPAC name: 6-isopropyl-3,3,7-trimethyldecane.

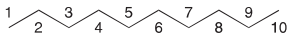
Solution

Follow three steps to derive a structure from a name.

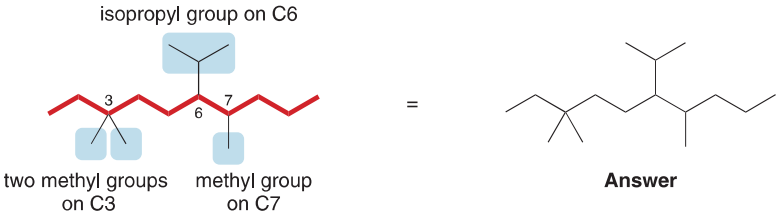
Step [1] Identify the parent name and functional group found at the *end* of the name.

decane ----→ **10** C's ----→ 

Step [2] Number the carbon skeleton in *either* direction.



Step [3] Add the substituents at the appropriate carbons.



Problem 4.9 Give the structure corresponding to each IUPAC name.

a. 3-methylhexane
b. 3,3-dimethylpentane
c. 3,5,5-trimethyloctane
d. 3-ethyl-4-methylhexane
e. 3-ethyl-5-isobutylnonane

Problem 4.10 Give the IUPAC name for each of the five constitutional isomers of molecular formula C_6H_{14} in Problem 4.3.

4.5 Naming Cycloalkanes

Cycloalkanes are named by using similar rules, but the prefix **cyclo-** immediately precedes the name of the parent.

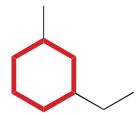
prefix + **cyclo-** + **parent** + **suffix**

What and where are the substituents? | How many C's are in the ring? | What is the functional group?

How To Name a Cycloalkane Using the IUPAC System

Step [1] **Find the parent cycloalkane.**

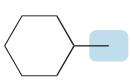
- Count the number of carbon atoms in the ring and use the parent name for that number of carbons. Add the prefix **cyclo-** and the suffix ***-ane*** to the parent name.



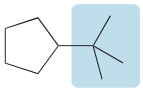
6 C's in the ring
cyclohexane

Step [2] **Name and number the substituents.**

- No number is needed to indicate the location of a single substituent.

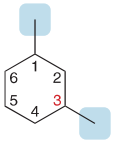


methylcyclohexane



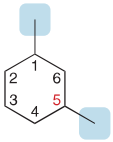
tert-butylcyclopentane

- For rings with more than one substituent, begin numbering at one substituent and proceed around the ring clockwise or counterclockwise to give the second substituent the lower number.



CH_3 groups at C1 and C3
The 2nd substituent has a lower number.

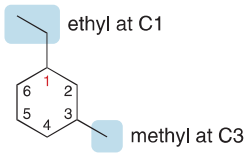
Correct: 1,3-dimethylcyclohexane



CH_3 groups at C1 and C5

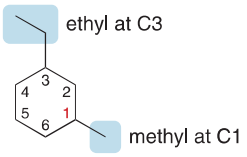
Incorrect: 1,5-dimethylcyclohexane

- With two different substituents, number the ring to assign the lower number to the substituents *alphabetically.*



earlier letter ⟶ lower number

Correct: 1-ethyl-3-methylcyclohexane

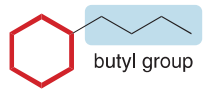


Incorrect: 3-ethyl-1-methylcyclohexane

When an alkane is composed of both a ring and a long chain, what determines whether a compound is named as an acyclic alkane or a cycloalkane? If the number of carbons in the ring is greater than or equal to the number of carbons in the longest chain, the compound is named as

a **cycloalkane,** as shown in Figure 4.2. Several examples of cycloalkane nomenclature are given in Figure 4.3.

Figure 4.2
Naming compounds containing both a ring and a chain of carbon atoms

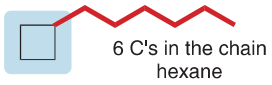


6 C's in the ring
cyclohexane

Name as a **cyclohexane** with a substituent.

butylcyclohexane

- Name the molecule as a substituted cycloalkane when it has more C's in the ring than any single alkyl substituent.



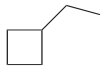
4 C's in the ring
cyclobutyl group

Name as a **hexane** with a substituent.

1-cyclobutylhexane

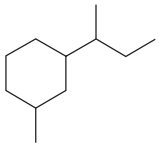
- Name the molecule as a substituted alkane when it has a carbon chain with more C's than the ring.

Figure 4.3
Examples of cycloalkane nomenclature



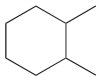
ethylcyclobutane

No number is needed with only one substituent.



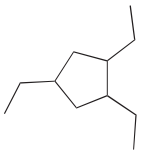
1-sec-butyl-3-methylcyclohexane

Assign the lower number to the 1st substituent alphabetically: the **b** of **b**utyl before the **m** of **m**ethyl.



1,2-dimethylcyclohexane

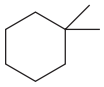
Number to give the 2nd CH_3 group the lower number: 1,2- not 1,6-.

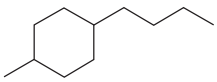


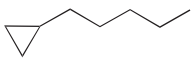
1,2,4-triethylcyclopentane

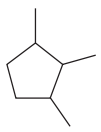
Number to give the 2nd CH_3CH_2 group the lower number: 1,2,4- not 1,3,4- or 1,3,5-.

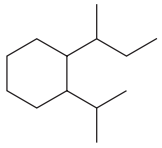
Problem 4.11 Give the IUPAC name for each compound.

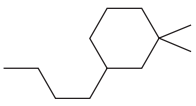
a. 

c. 

e. 

b. 

d. 

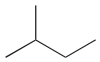
f. 

Problem 4.12 Give the structure corresponding to each IUPAC name.

a. 1,2-dimethylcyclobutane
b. 1,1,2-trimethylcyclopropane
c. 4-ethyl-1,2-dimethylcyclohexane
d. 1-*sec*-butyl-3-isopropylcyclopentane
e. 1,1,2,3,4-pentamethylcycloheptane

4.6 Common Names

Some organic compounds are identified using **common names** that do not follow the IUPAC system of nomenclature. Many of these names were given to molecules long ago, before the IUPAC system was adopted. These names are still widely used. For example, isopentane, an older name for 2-methylbutane, is still allowed by IUPAC rules. We will follow the IUPAC system except in cases in which a common name is widely accepted.



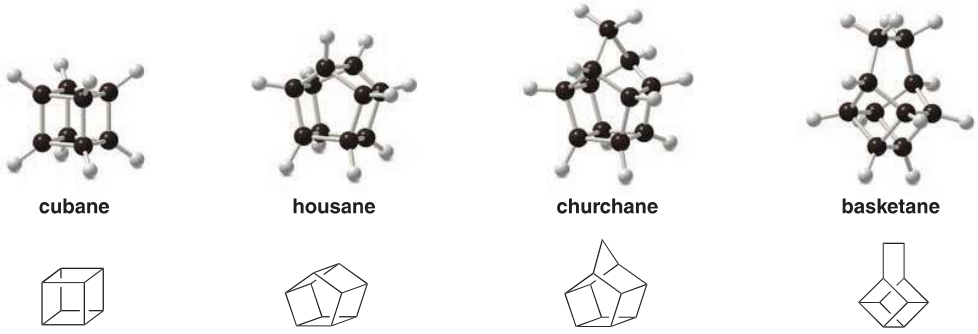
isopentane or 2-methylbutane

dodecahedrane

In the past several years organic chemists have attempted to synthesize some unusual cycloalkanes not found in nature. **Dodecahedrane,** a beautifully symmetrical compound composed of 12 five-membered rings, is one such molecule. It was first prepared at The Ohio State University in 1982. The IUPAC name for dodecahedrane is undecacyclo[9.9.0.0^{2,9}.0^{3,7}.0^{4,20}.0^{5,18}.0^{6,16}.0^{8,15}.0^{10,14}.0^{12,19}.0^{13,17}]-icosane, a name so complex that few trained organic chemists would be able to identify its structure.

Because these systematic names are so unwieldy, organic chemists often assign a name to a polycyclic compound that is more descriptive of its shape and structure. Dodecahedrane is named because its 12 five-membered rings resemble a dodecahedron. Figure 4.4 shows the names and structures of several other cycloalkanes whose names were inspired by the shape of their carbon skeletons. All the names end in the suffix ***-ane,*** indicating that they refer to alkanes.

Figure 4.4
Common names for some polycyclic alkanes



For a more comprehensive list of unusual polycyclic alkanes (including windowpane, davidane, catenane, propellane, and many others), see *Organic Chemistry: The Name Game* by Alex Nickon and Ernest Silversmith, Pergamon Press, 1987.

4.7 Fossil Fuels

Natural gas is odorless. The smell observed in a gas leak is due to minute amounts of a sulfur additive such as methanethiol, CH_3SH, which provides an odor for easy detection.

Many alkanes occur in nature, primarily in natural gas and petroleum. Both of these fossil fuels serve as energy sources, formed from the degradation of organic material long ago.

Natural gas is composed largely of **methane** (60% to 80% depending on its source), with lesser amounts of ethane, propane, and butane. These organic compounds burn in the presence of oxygen, releasing energy for cooking and heating.

Petroleum is a complex mixture of compounds, most of which are hydrocarbons containing 1–40 carbon atoms. Distilling crude petroleum, a process called **refining,** separates it into usable