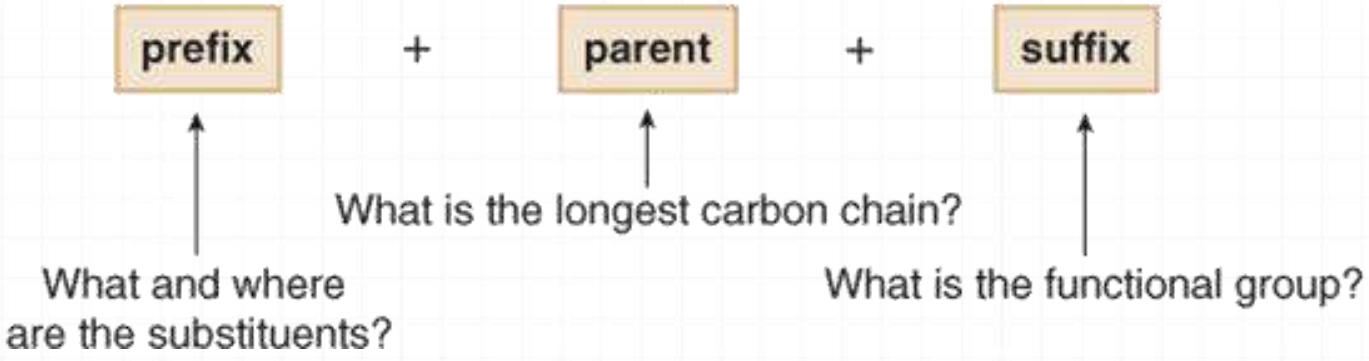
Alkanes - Nomenclature

The name of every organic molecule has 3 parts:

1. **The parent name indicates the number of carbons in the longest continuous chain.**
2. **The suffix indicates what functional group is present.**
3. **The prefix tells us the identity, location, and number of substituents attached to the carbon chain.**



Alkanes - Nomenclature

Parent – Longest straight carbon chain

TABLE 4.1 Summary: Straight-Chain Alkanes

Number of C atoms	Molecular formula	Name (*n*-alkane)	Number of constitutional isomers
1	CH_4	methane	—
2	C_2H_6	ethane	—
3	C_3H_8	propane	—
4	C_4H_{10}	butane	2
5	C_5H_{12}	pentane	3
6	C_6H_{14}	hexane	5
7	C_7H_{16}	heptane	9
8	C_8H_{18}	octane	18
9	C_9H_{20}	nonane	35
10	$C_{10}H_{22}$	decane	75
20	$C_{20}H_{42}$	eicosane	366,319

Alkanes - Nomenclature

Suffix – Our first functional group is alkane, so the suffix is –ane

For later functional groups we will drop the –ane root suffix for others

Alkane chain	# Carbons	Name
CH_4	1	methane
CH_3CH_3	2	ethane
$CH_3CH_2CH_3$	3	propane
$CH_3CH_2CH_2CH_3$	4	butane
$CH_3CH_2CH_2CH_2CH_3$	5	pentane
$CH_3CH_2CH_2CH_2CH_2CH_3$	6	hexane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$	7	heptane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	8	octane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	9	nonane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	10	decane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	11	undecane
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	12	dodecane

Alkanes - Nomenclature

Prefix – Our substituents will be branches in the alkane structure

A branch is another alkane minus one hydrogen – **an alkyl group**

Example – if CH_3- is a branch on a longer chain:

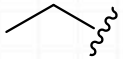
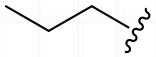
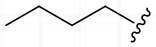
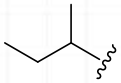
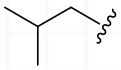
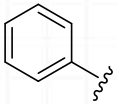
CH_3- is CH_4 minus 1 hydrogen

Since it is a side chain it will replace the –ane suffix with –yl

CH_3- is a methyl group

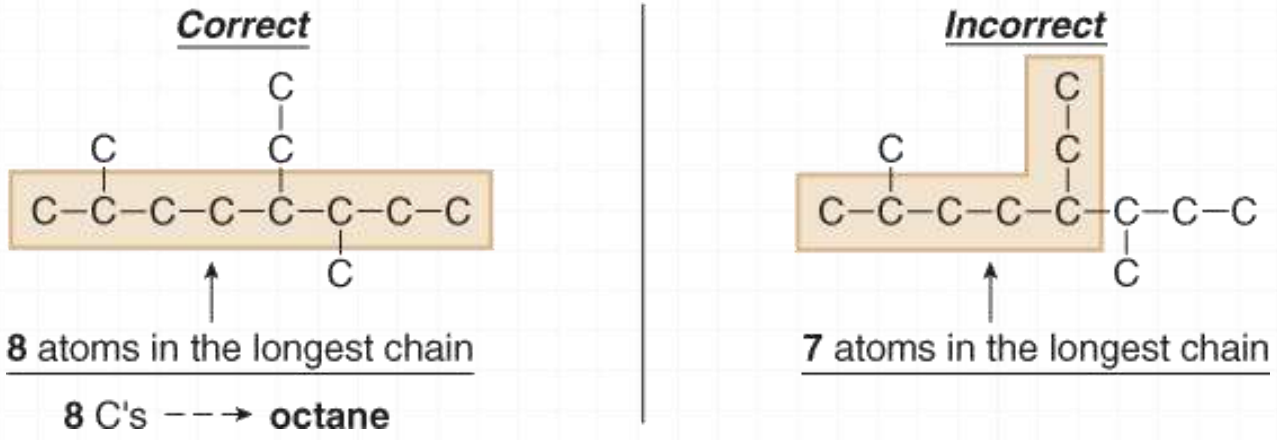
Alkanes - Nomenclature

Prefixes -

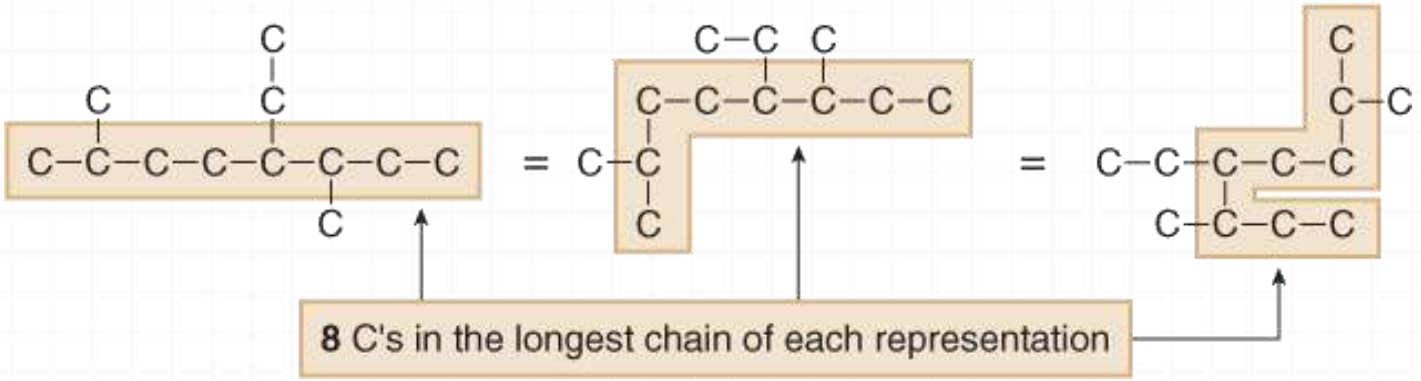
Alkyl group	Structure	IUPAC name	Abbreviation
CH_3-	CH_3-	methyl	Me-
CH_3CH_2-		ethyl	Et-
$CH_3CH_2CH_2$-		*n*-propyl	*n*-Pr
CH_3CHCH_3		isopropyl or *i*-propyl	*i*-Pr
$CH_3CH_2CH_2CH_2$-		*n*-butyl	*n*-Bu
$CH_3CH_2CHCH_3$		*sec*-butyl	*s*-Bu
$(CH_3)_2CHCH_2$-		isobutyl or *i*-butyl	*i*-Bu
$(CH_3)_3C$-		*tert*-butyl or *t*-butyl	*t*-Bu
C_6H_5-		phenyl	Ph

Alkanes - Nomenclature

1. Find the parent carbon chain and add the suffix.

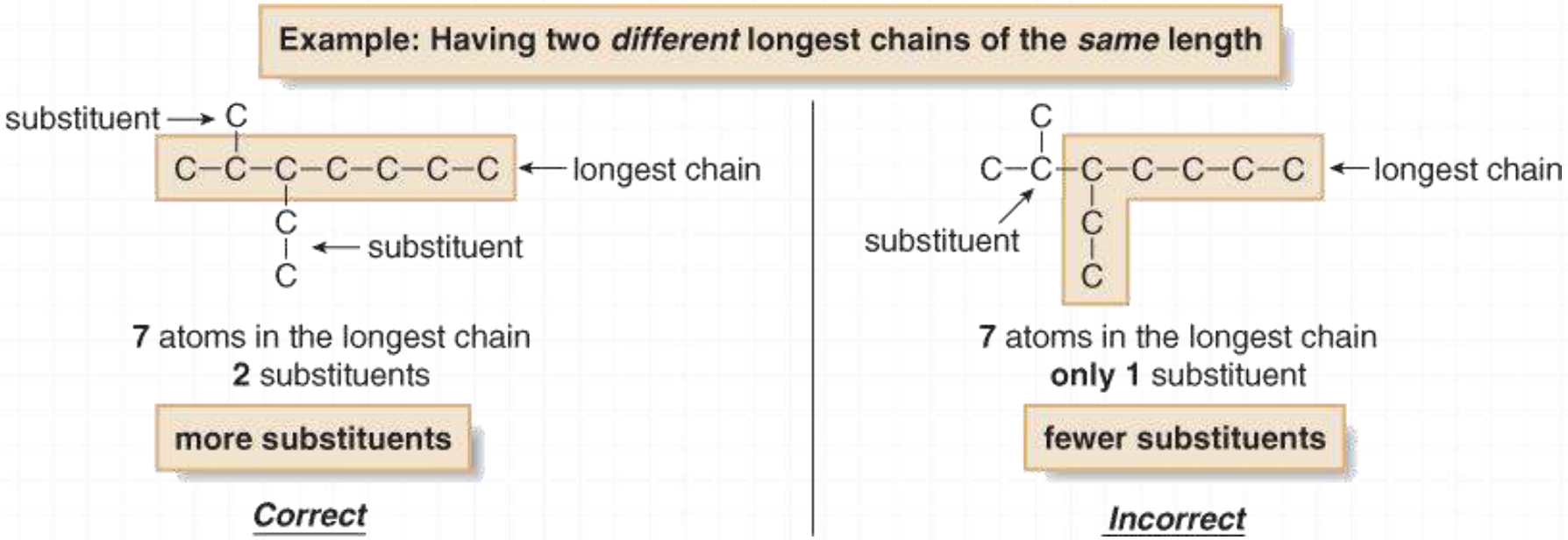


Note that it does not matter if the chain is straight or it bends.



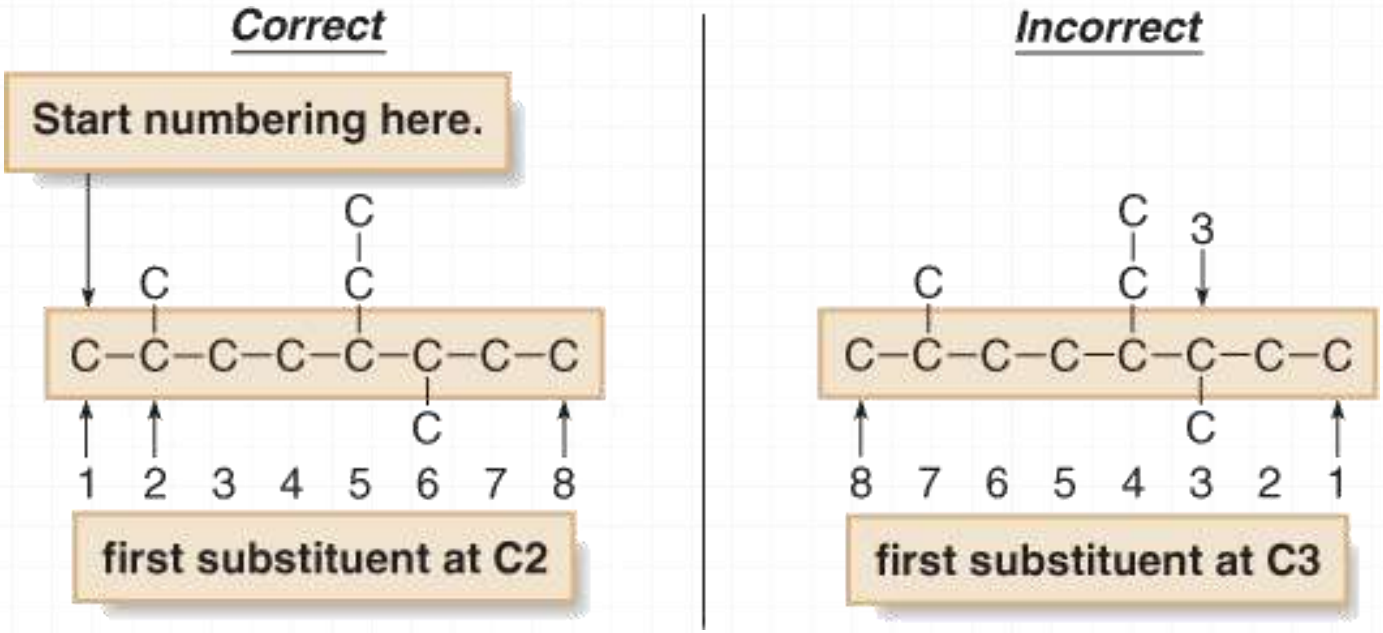
Alkanes - Nomenclature

Also note that 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 have seven C atoms. We circle the longest continuous chain as shown in the diagram on the left, since this results in the greater number of substituents.



Alkanes - Nomenclature

2. Number the atoms in the carbon chain to give the first substituent the lowest number.

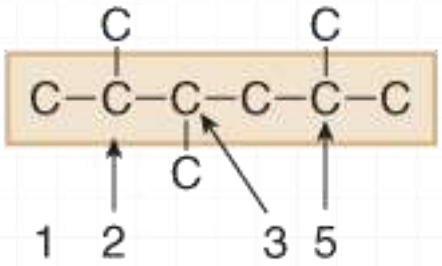


Alkanes - Nomenclature

If the first substituent is the same distance from both ends, number the chain to give the second substituent the lower number.

Example: Giving a lower number to the *second* substituent

Numbering from *left* to right

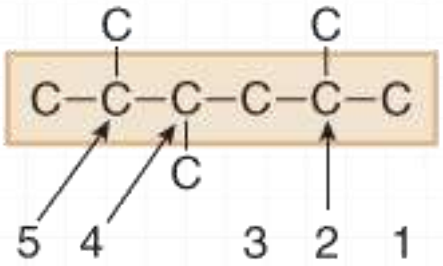


CH_3 groups at C2, **C3,** and C5.

The second substituent has a lower number.

Correct

Numbering from *right* to left



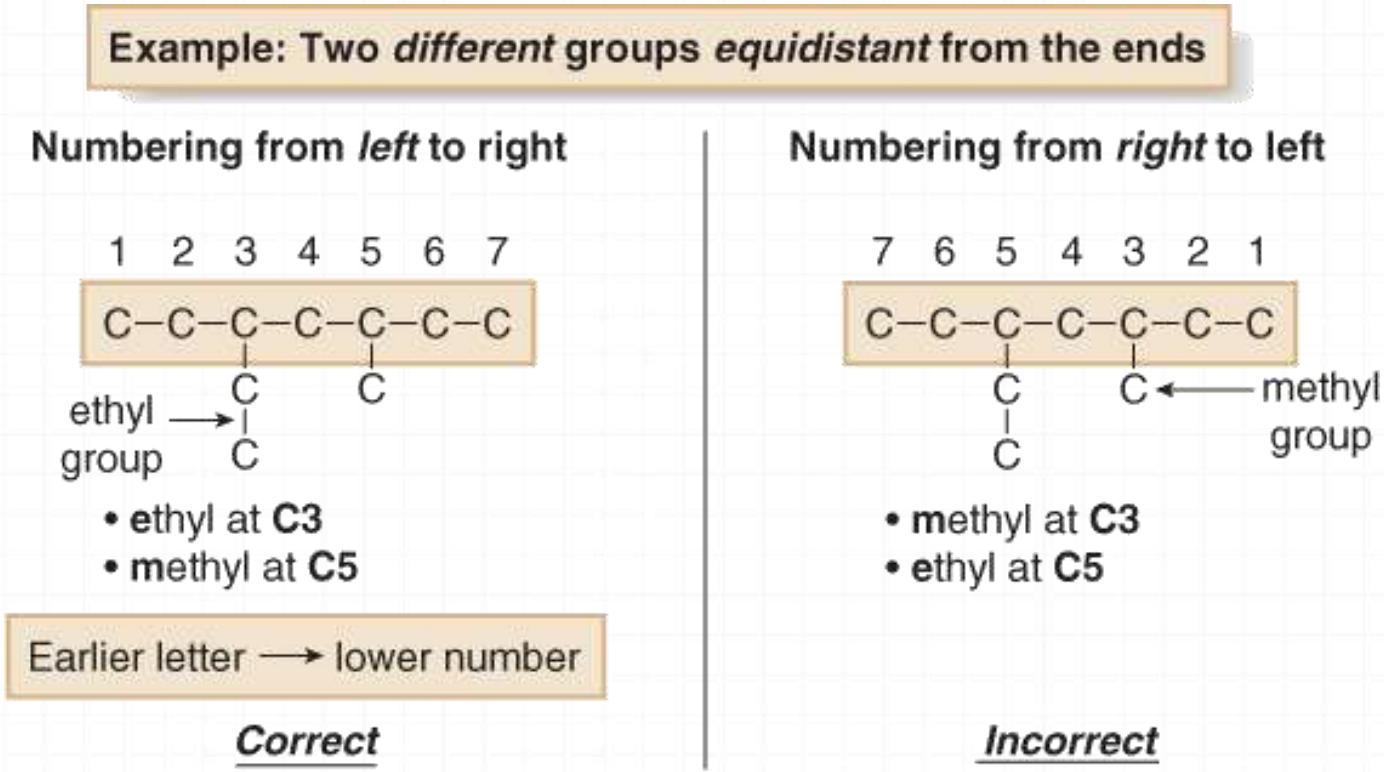
CH_3 groups at C2, **C4,** and C5.

higher number

Incorrect

Alkanes - Nomenclature

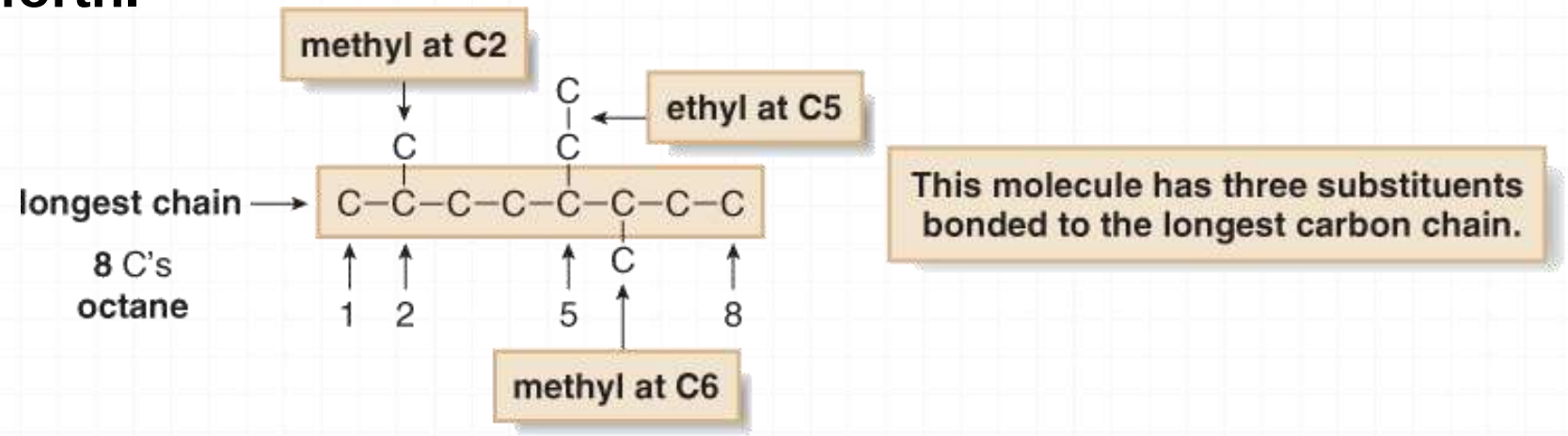
When numbering a carbon chain results in the same numbers from either end of the chain, assign the lower number alphabetically to the first substituent.



Alkanes - Nomenclature

3. Name and number the substituents.

- **Name the substituents as alkyl groups.**
- **Every carbon belongs to either the longest chain or a substituent, 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.**

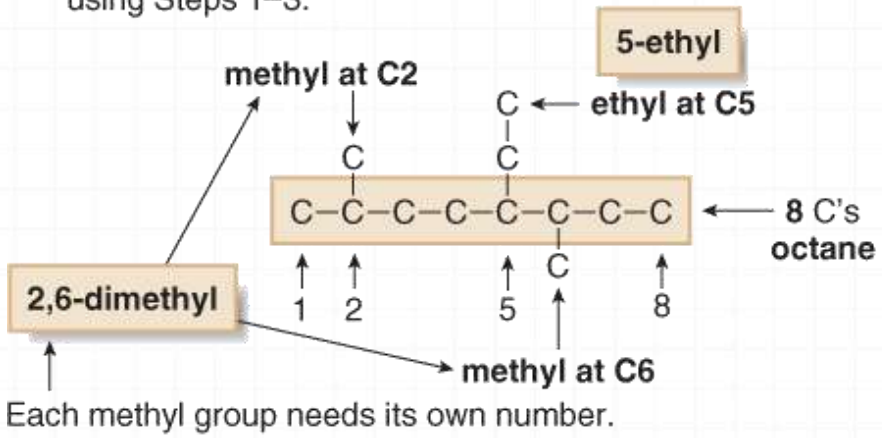


Alkanes - Nomenclature

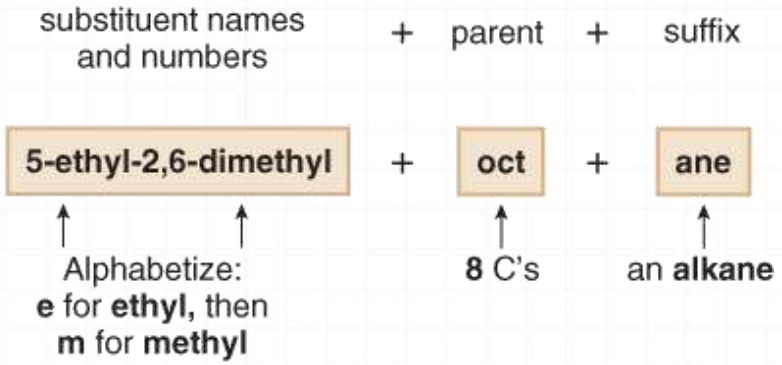
4. Combine substituent names and numbers + parent and suffix.

- **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.**
- **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 and commas.**

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

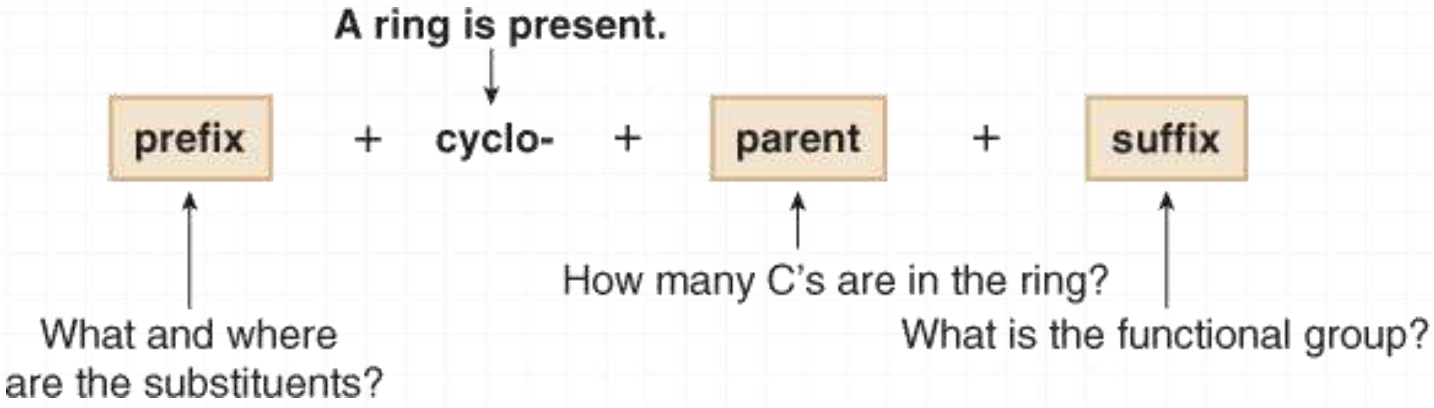


[2] Then, put the pieces of the name together.

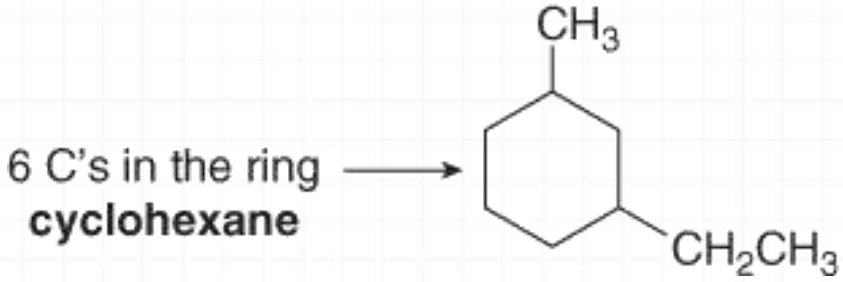


Alkanes - Nomenclature

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

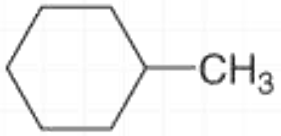


1. Find the parent cycloalkane.

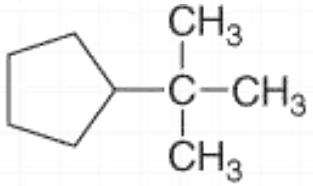


Alkanes - Nomenclature

2. Name and number the substituents. No number is needed to indicate the location of a single substituent.



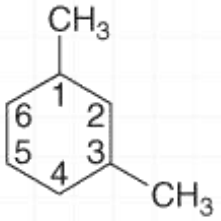
methylcyclohexane



tert-butylcyclopentane

For rings with more than one substituent, begin numbering at one substituent and proceed around the ring to give the second substituent the lowest number.

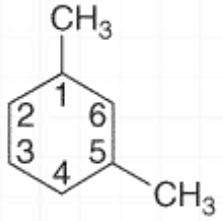
numbering clockwise



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

Correct: **1,3-dimethylcyclohexane**

numbering counterclockwise



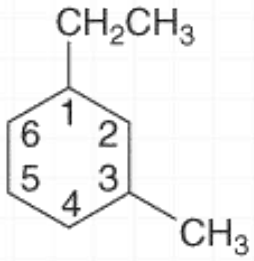
CH_3 groups at C1 and **C5**

Incorrect: 1,5-dimethylcyclohexane

Alkanes - Nomenclature

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

Begin numbering at the ethyl group.

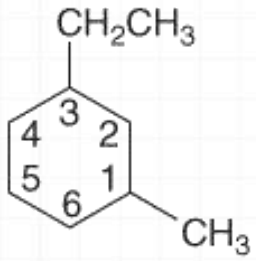


- **e**thyl group at **C1**
- **m**ethyl group at **C3**

earlier letter → lower number

Correct: **1-ethyl-3-methylcyclohexane**

Begin numbering at the methyl group.



- **m**ethyl group at **C1**
- **e**thyl group at **C3**

Incorrect: 3-ethyl-1-methylcyclohexane

Note the special case of an alkane composed of both a ring and a long chain. 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.

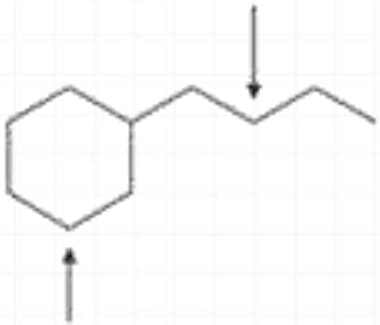
Alkanes - Nomenclature

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

Contrast two different examples

more carbons in the ring

4 C's in the chain — a **butyl** group



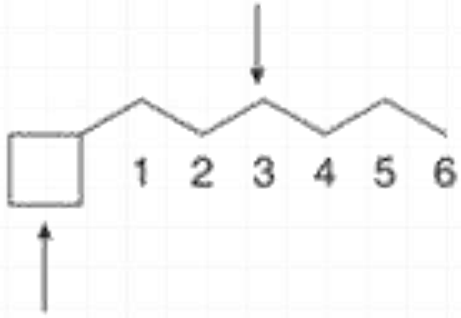
6 C's in the ring—**cyclohexane**

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

Answer: butylcyclohexane

more carbons in the chain

6 C's in the chain — a **hexane**



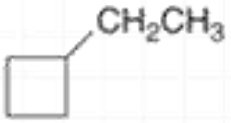
4 C's in the ring—a **cyclobutyl** group

Name as a *hexane* with a substituent.

Answer: 1-cyclobutylhexane

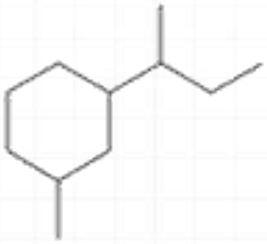
Alkanes - Nomenclature

Figure 4.3 Examples of cycloalkane nomenclature



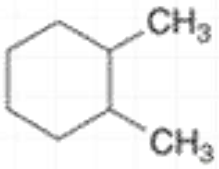
ethylcyclobutane

No number is needed with only one substituent.



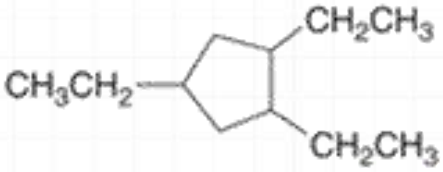
1-*sec*-butyl-3-methylcyclohexane

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

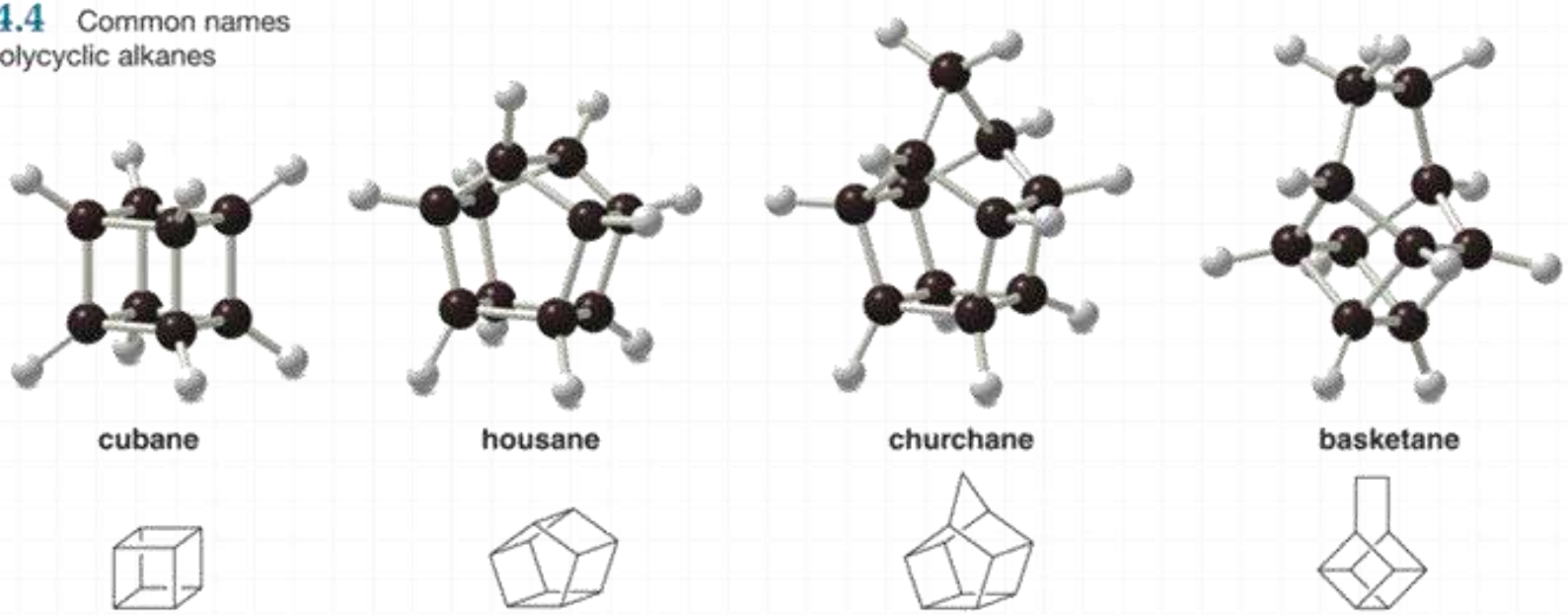
Number to give the 2nd CH_3CH_2 group the lower number: 1,2,4- not 1,3,4- or 1,3,5-.

Alkanes - Nomenclature

Nomenclature—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 long ago before the IUPAC system was adopted, and are still widely used. Additionally, some names are descriptive of shape and structure, like those below:

Figure 4.4 Common names for some polycyclic alkanes



Other Functional Groups - Nomenclature

The IUPAC rules for all other functional groups will differ only by the following:

1. Suffix will change to reflect functional group

2. Some functional groups have priority over others

3. We actually cover the functional groups in 210/212 in order of this priority (except Amines, Ch 22):

For now: Alcohol > Alkyne > Alkene > alkane=alkyl halide

4. The longest chain must contain the suffix functional group – even if not the longest chain overall

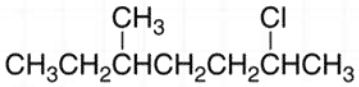
5. Numbering gives this functional group the lowest number – even if there are other groups that would be lower

6. If an alkene has *stereochemistry*, it must be specified in the prefix

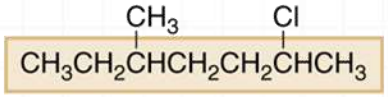
Alkyl Halides - Nomenclature

HOW TO Name an Alkyl Halide Using the IUPAC System

Example Give the IUPAC name of the following alkyl halide:



Step [1] Find the parent carbon chain containing the halogen.



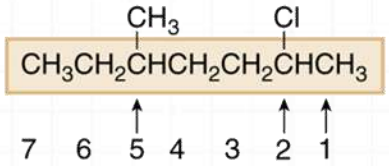
7 C's in the longest chain

7 C's ----→ **heptane**

- Name the parent chain as an ***alkane,*** with the halogen as a substituent bonded to the longest chain.

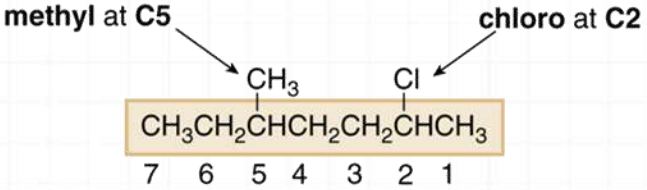
Step [2] Apply all other rules of nomenclature.

a. **Number** the chain.



- Begin at the end nearest the first substituent, either alkyl or halogen.

b. **Name** and **number** the substituents.



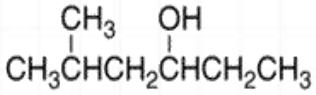
c. **Alphabetize: c** for **c**hloro, then **m** for **m**ethyl.

ANSWER: 2-chloro-5-methylheptane

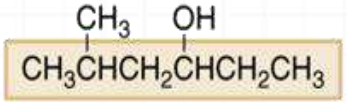
Alcohols - Nomenclature

HOW TO Name an Alcohol Using the IUPAC System

Example Give the IUPAC name of the following alcohol:



Step [1] Find the longest carbon chain containing the carbon bonded to the OH group.



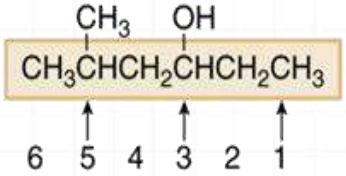
6 C's in the longest chain

6 C's → hexan*e* → hexan*ol*

- Change the ***-e*** ending of the parent alkane to the suffix ***-ol.***

Step [2] Number the carbon chain to give the OH group the lower number, and apply all other rules of nomenclature.

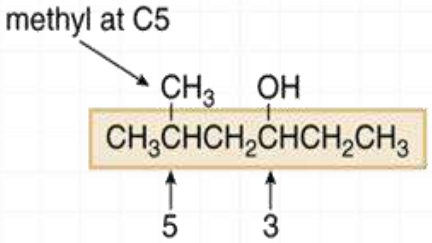
a. **Number** the chain.



- Number the chain to put the OH group at C3, not C4.

3-hexanol

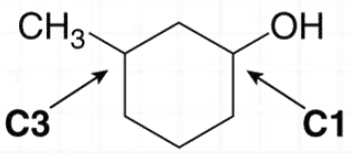
b. **Name** and **number** the substituents.



Answer: 5-methyl-3-hexanol

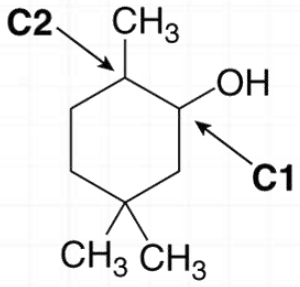
Alcohols - Nomenclature

- When an OH group is bonded to a ring, the ring is numbered beginning with the OH group.
- Because the functional group is at C1, the 1 is usually omitted from the name.
- The ring is then numbered in a clockwise or counterclockwise fashion to give the *next* substituent the lowest number.



3-methylcyclohexanol

[The OH group is at C1; the second substituent (CH_3) gets the lower number.]

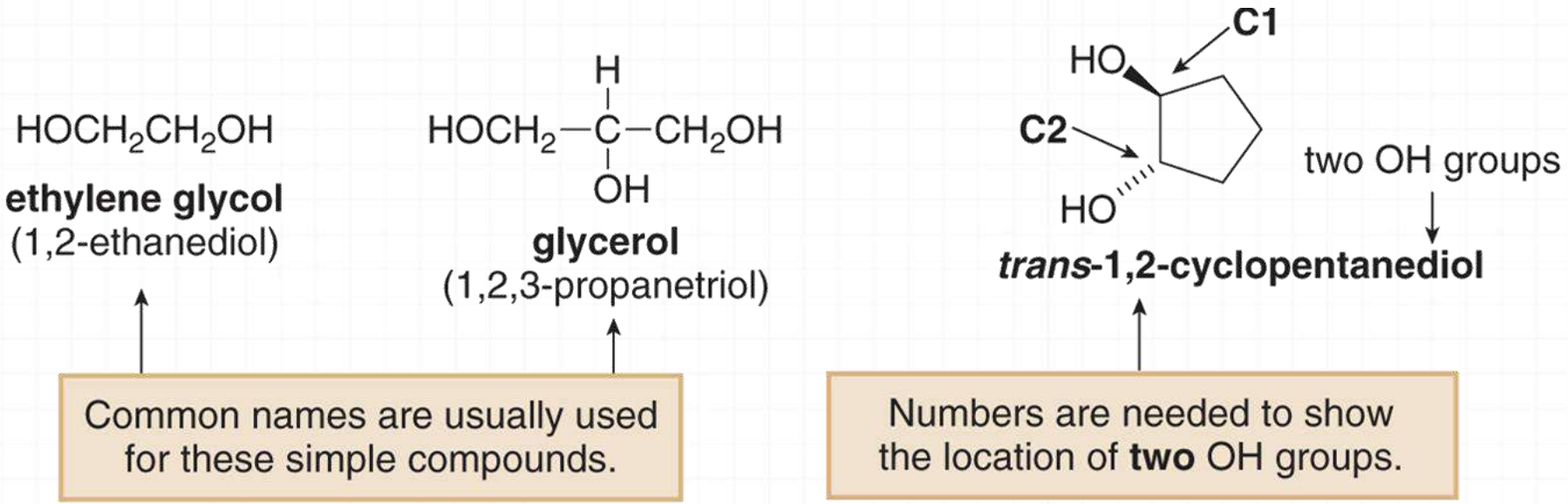


2,5,5-trimethylcyclohexanol

[The OH group is at C1; the second substituent (CH_3) gets the lower number.]

Alcohols - Nomenclature

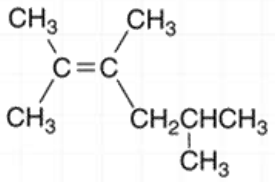
- Compounds with two hydroxyl groups are called diols or glycols.
- Compounds with three hydroxyl groups are called triols.



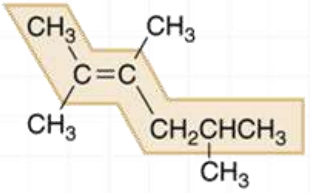
Alkenes - Nomenclature

HOW TO Name an Alkene

Example Give the IUPAC name of the following alkene:



Step [1] Find the longest chain that contains *both* carbon atoms of the double bond.



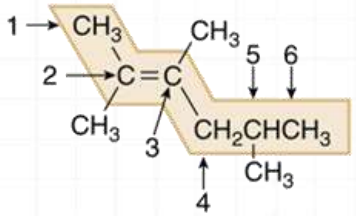
6 C's in the longest chain

hex*ane* ----→ **hex*ene***

- Change the ***-ane*** ending of the parent alkane to ***-ene.***

Step [2] Number the carbon chain to give the double bond the lower number, and apply all other rules of nomenclature.

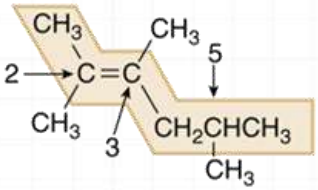
a. **Number** the chain, and name using the ***first* number** assigned to the C=C.



- Number the chain to put the C=C at C2, not C4.

2-hexene

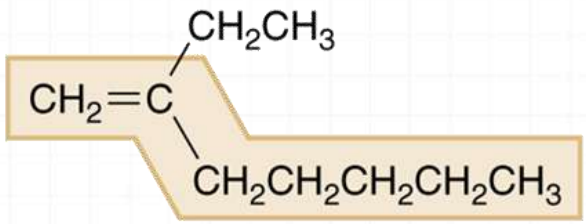
b. **Name** and **number** the substituents.



three methyl groups at C2, C3, and C5

Answer: 2,3,5-trimethyl-2-hexene

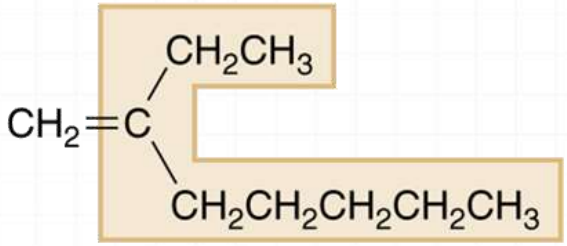
Alkenes - Nomenclature



7 C's ----→ heptene

Both C's of the C=C are contained in this long chain.

***Correct:* 2-ethyl-1-heptene**

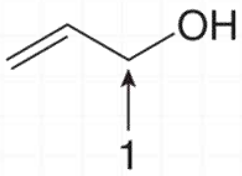


8 C's

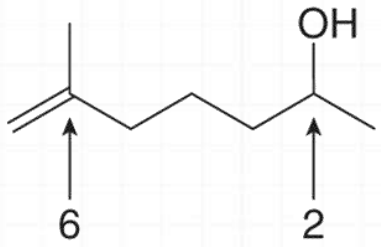
Both C's of the C=C are NOT contained in this long chain.

Incorrect

- Compounds that contain both a double bond and a hydroxy group are named as alkenols and the chain (or ring) is numbered to give the OH group the lower number.



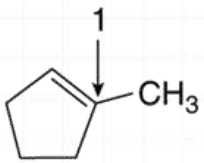
2-propen-1-ol



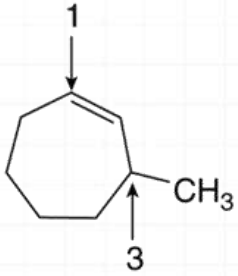
6-methyl-6-hepten-2-ol

Alkenes - Nomenclature

- Compounds with two double bonds are named as dienes by changing the “-ane” ending of the parent alkane to the suffix “-adiene”.
- Compounds with three double bonds are named as trienes, and so forth.
- In naming cycloalkenes, the double bond is located between C1 and C2, and the “1” is usually omitted in the name.
- The ring is numbered clockwise or counterclockwise to give the first substituent the lower number.

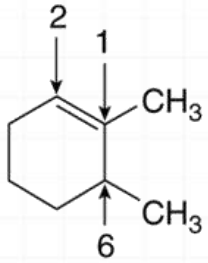


1-methylcyclopentene



3-methylcycloheptene

Number clockwise beginning at the C=C and place the CH_3 at C3.



1,6-dimethylcyclohexene

Number counterclockwise beginning at the C=C and place the first CH_3 at C1.

Alkenes - Nomenclature

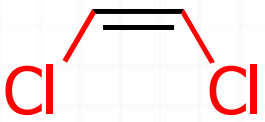
Disubstituted Alkenes - Stereochemistry:

There is no free rotation about the π-bond

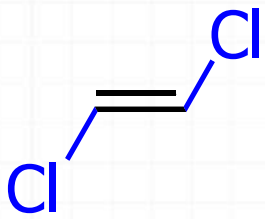
cis- vs. *trans*-

- *cis:* two identical or substantial groups on the same side of C=C

- *trans:* two identical or substantial groups on the opposite side of C=C



cis-1,2-Dichloroethene



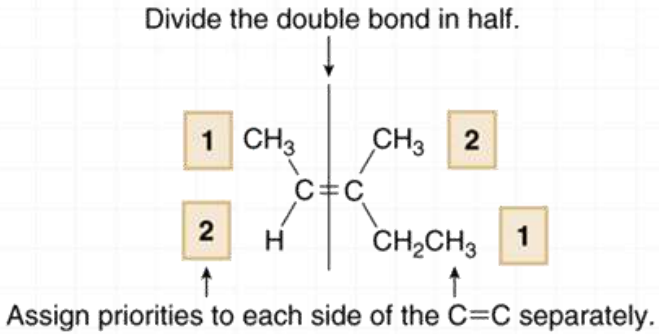
trans-1,2-Dichloroethene

Alkenes - Nomenclature

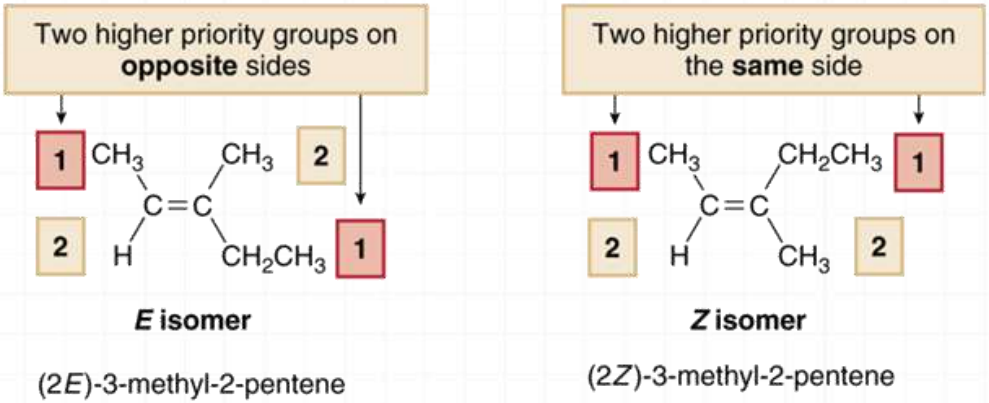
HOW TO Assign the Prefixes *E* and *Z* to an Alkene

Step [1] Assign priorities to the two substituents on each end of the C=C by using the priority rules for *R,S* nomenclature (Section 5.6).

- Divide the double bond in half, and assign the numbers **1** and **2** to indicate the relative priority of the two groups on each end—the higher priority group is labeled **1,** and the lower priority group is labeled **2.**



Step [2] Assign *E* or *Z* based on the location of the two higher priority groups (1).



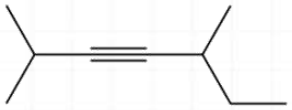
- The ***E*** isomer has the two higher priority groups on the **opposite sides.**
- The ***Z*** isomer has the two higher priority groups on the **same side.**

Alkynes - Nomenclature

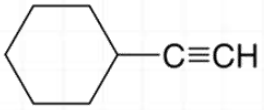
- Alkynes are named in the same general way that alkenes are named.
- In the IUPAC system, change the –*ane* ending of the parent alkane name to the suffix –*yne*.
- Choose the longest continuous chain that contains both atoms of the triple bond and number the chain to give the triple bond the lower number.

Alkynes - Nomenclature

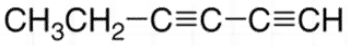
- Compounds with two triple bonds are named as diynes, those with three are named as triynes and so forth.
- Compounds with both a double and triple bond are named as enynes.
- The chain is numbered to give the first site of unsaturation (either C=C or C≡C) the lower number.



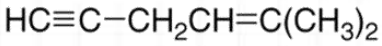
2,5-dimethyl-3-heptyne



ethynylcyclohexane



1,3-hexadiyne



5-methyl-4-hexen-1-yne