7.4: NAMING ALKENES

OBJECTIVES

After completing this section, you should be able to

- provide the correct IUPAC name for an acyclic or cyclic alkene, given its Kekulé, condensed or shorthand structure.
- draw the Kekulé, condensed or shorthand structure of an alkene (cyclic or acyclic), given its IUPAC name.
- give the IUPAC equivalent of the following trivial names: ethylene, propylene, isobutylene and isoprene.
- draw the structure of a vinyl (ethenyl) and allyl (2-propenyl) group, and use these names in alkene nomenclature.

STUDY NOTES

This course uses IUPAC nomenclature; therefore, you need not usually memorize a large number of trivial names. However, you will encounter some trivial names so frequently in books and articles that they soon become familiar.

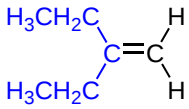
An alkene that can exhibit geometric isomerism has not been properly named unless its name specifies whether the double bond (or bonds) is (or are) cis or trans. The most effective way of giving this information is discussed, and more details of cis and trans follow in Section 7.4.

Alkenes contain carbon-carbon double bonds and are unsaturated hydrocarbons with the molecular formula is C_nH_{2n}; this is also the same molecular formula as cycloalkanes. The parent chain of an alkene is the longest chain containing both carbon atoms of the double bond. Alkenes are named by dropping the **-ane** ending of the parent and adding **-ene**. Also, the position of double bond in the parent chain of the alkene is indicated with a number.

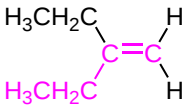
THE BASIC RULES FOR NAMING ALKENES

For straight chain alkenes, it is the same basic rules as nomenclature of alkanes apply except the **-ane** suffix is changed to **-ene**.

1) Find the longest carbon chain that contains both carbons of the double bond.

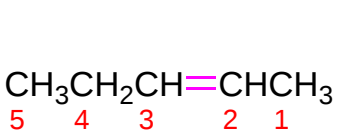


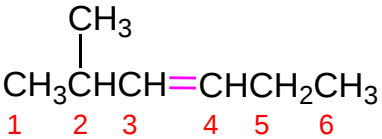
This compound is NOT named as an pentene



This compound is named as a butene because the double bond is contained in the four carbon chain

2) Start numbering from the end of the parent chain which gives the lowest possible number to the double bond. If the double bond is equidistant from both ends of the parent chain, number from the end which gives the substituents the lowest possible number. The double bond in cycloalkenes do not need to number because it is understood that they are in the one position.



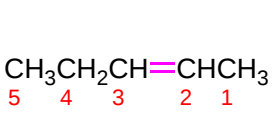


3) Place the location number of the double bond directly before the parent name. The location number indicates the position of the first carbon of the double bond. Add substituents and their position to the alkene as prefixes. Remember substituents are written in alphabetical order.

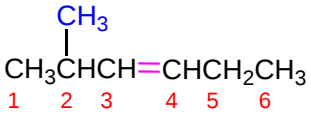
The presence of multiple double bonds is indicated by using the appropriate suffix such as **-diene**, **-triene**, ect. Each of the multiple bonds receives a location number. Also, only **-ne** is removed from the parent alkane chain name leaving an "a" in the name.

Overall, the name of an alkene should look like:

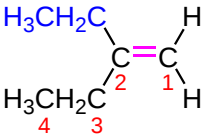
(Location number of substituent)-(Name of substituent)-(Location number of double bond)-(Name of parent chain) + ene



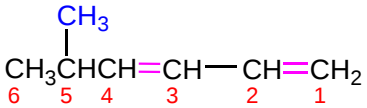
2-Pentene



2-Methyl-3-hexene



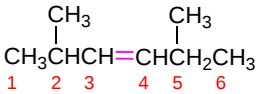
3-Ethyl-1-butene

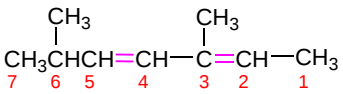


5-Methyl-1,3-hexadiene

NEWER IUPAC NOMENCLATURE

In 1993 IUPAC updated their naming recommendation to place the location number of the double bond before the -ene suffix of alkene names. The provides names such as hex-2-ene rather than 2-hexene. The newer system is slowly being accepted so it may occasionally be encountered.

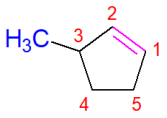




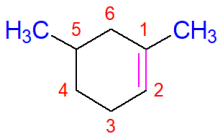
Older Numbering System:	**2,5-Dimethyl-3-hexene**	**5-Methyl-1,3-hexadiene**
Newer Numbering System:	**2,5-Dimethylhex-3-ene**	**5-Methylhexa-1,3-diene**

NAMING CYCLOALKENES

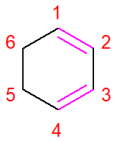
Because there are no chain ends in cycloalkenes, the double bond is assumed to numbered C1 and C2 and its location number is not required in the name. The direction of the numbering is determined by which will give the substituent closest to the double bond the lowest number. If multiple double bonds are present, it may be necessary to include their location numbers in the name. One of the double bonds will be number C1 and C2 and the numbering direction is determined by which gives the remaining double bonds the lowest possible number.



3-Methylcyclopent-1-ene



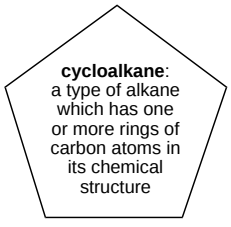
1,5-Dimethylcyclohexene



1,3-Cyclohexadiene
(New:Cyclohexa-1,3-diene)

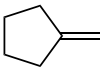
ENDOCYCLIC VS. EXOCYCLIC ALKENES

Endocyclic double bonds have both carbons in the ring and exocyclic double bonds have only one carbon as part of the ring.



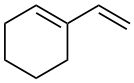
Cyclopentene is an example of an endocyclic double bond.

Methylenecylopentane is an example of an exocyclic double bond.



Name the following compounds...

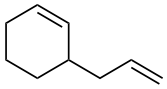
1-methylcyclobutene. The methyl group places the double bond. It is correct to also name this compound as 1-methylcyclobut-1-ene.



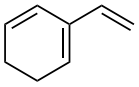
1-ethenylcyclohexene, the methyl group places the double bond. It is correct to also name this compound as 1-ethenylcyclohex-1-ene. A common name would be 1-vinylcyclohexene.

Try to draw structures for the following compounds...

- 3-allylcyclohex-1-ene

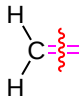


- 2-vinyl-1,3-cyclohexadiene

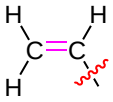


COMMON NAMES OF ALKENE FRAGMENTS

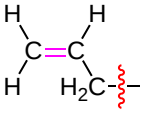
Some alkene containing fragments have common names which should be recognized. These common names can be used to simplify naming much the alkyl fragments discussed in **Section: 3.3**. Some of these fragments are the methylene group (H_2C=), the vinyl group (H_2C=CH-), and the allyl group (H_2C=CH-CH_2-).



Methylene Group

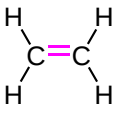


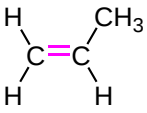
Vinyl Group

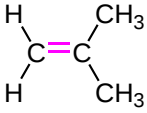


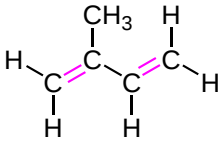
Allyl Group

In addition, the common name some small alkene compounds are still accepted by IUPAC. It is important to be able to identify them.





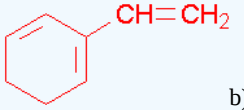


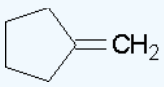


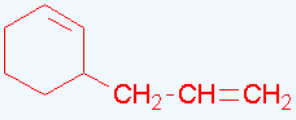
Common Name:	**Ethylene**	**Propylene**	**Isobutylene**	**Isoprene**
IUPAC Name:	**Ethene**	**Propene**	**2-Methylpropene**	**2-Methyl-1,3-butadiene**

? EXERCISE 7.4.1

Name the following compounds using common fragment names.

a) 

b) 

C) 

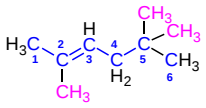
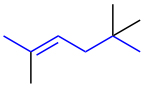
Answer

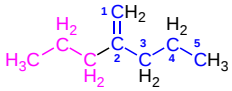
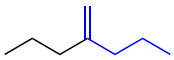
a) 2-Vinyl-cyclohexa-1,3-diene

b) Methylenecylopentane

c) 3-Allylcyclohex-1-ene

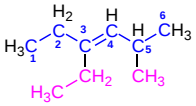
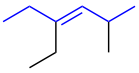
EXAMPLES

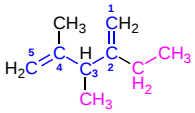
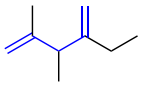
(1)  ≡  ≡ $(CH_3)_2C{=}CHCH_2C(CH_3)_3$
2,5,5-trimethyl-2-hexene

(2)  ≡  ≡ $(CH_3CH_2CH_2)_2C{=}CH_2$
2-propyl-1-pentene

Both these compounds have double bonds, making them alkenes. In example (1) the longest chain consists of six carbons, so the root name of this compound will be hexene. Three methyl substituents (colored red) are present. Numbering the six-carbon chain begins at the end nearest the double bond (the left end), so the methyl groups are located on carbons 2 & 5. The IUPAC name is therefore: 2,5,5-trimethyl-2-hexene.

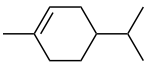
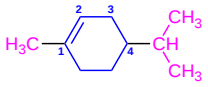
In example (2) the longest chain incorporating both carbon atoms of the double bond has a length of five. There is a seven-carbon chain, but it contains only one of the double bond carbon atoms. Consequently, the root name of this compound will be pentene. There is a propyl substituent on the inside double bond carbon atom (#2), so the IUPAC name is: 2-propyl-1-pentene.

(3)  ≡  ≡ $(CH_3CH_2)_2C{=}CHCH(CH_3)_2$
4-ethyl-2-methyl-3-hexene

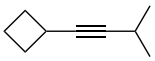
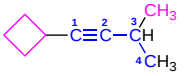
(4)  ≡  ≡ $CH_2{=}C(CH_3)CH(CH_3)C(C_2H_5){=}CH_2$
2-ethyl-3,4-dimethyl-1,4-pentadiene

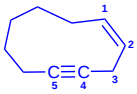
The double bond in example (3) is located in the center of a six-carbon chain. The double bond would therefore have a locator number of 3 regardless of the end chosen to begin numbering. The right hand end is selected because it gives the lowest first-substituent number (2 for the methyl as compared with 3 for the ethyl if numbering were started from the left). The IUPAC name is assigned as shown.

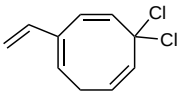
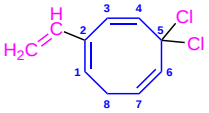
Example (4) is a diene (two double bonds). Both double bonds must be contained in the longest chain, which is therefore five- rather than six-carbons in length. The second and fourth carbons of this 1,4-pentadiene are both substituted, so the numbering begins at the end nearest the alphabetically first-cited substituent (the ethyl group).

(5)  ≡  ≡ 4-isopropyl-1-methylcyclohexene

4-isopropyl-1-methylcyclohex-1-ene

(6)  ≡  ≡ 1-cyclobutyl-3-methyl-1-butyne

(7)  ≡  ≡ 1-cyclodecen-4-yne

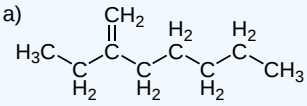
(8)  ≡  ≡ 5,5-dichloro-2-vinyl-1,3,6-cyclooctatriene

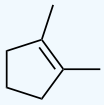
These examples include rings of carbon atoms as well as some carbon-carbon triple bonds. Example (6) is best named as an alkyne bearing a cyclobutyl substituent. Example (7) is simply a ten-membered ring containing both a double and a triple bond. The double bond is cited first in the IUPAC name, so numbering begins with those two carbons in the direction that gives the triple bond carbons the lowest locator numbers. Because of the linear geometry of a triple bond, a-ten membered ring is the smallest ring in which this functional group is easily accommodated. Example (8) is a cyclooctatriene (three double bonds in an eight-membered ring). The numbering must begin with one of the end carbons of the conjugated diene moiety (adjacent double bonds), because in this way the double bond carbon atoms are assigned the

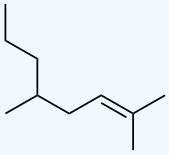
smallest possible locator numbers (1, 2, 3, 4, 6 & 7). Of the two ways in which this can be done, we choose the one that gives the vinyl substituent the lower number.

EXERCISE 7.4.2

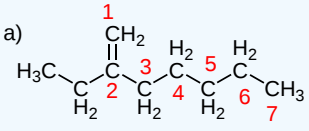
Name the following alkenes.

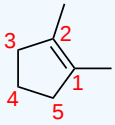
a) 

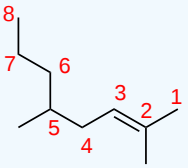
b) 

c) 

Answer

a) 

b) 

c) 

a) 2-ethylhept-1-ene or 2-ethyl-1-heptene

b) 1,2-dimethylcyclohept-1-ene

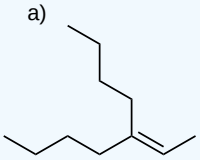
c) 2,5-dimethyloct-2-ene or 2,5-dimethyl-1-octene

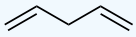
EXERCISE 7.4.3

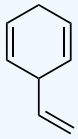
Draw structures for the following compounds from the given names.

a. 3-butylhept-2-ene (3-butyl-2-heptene)
b. 1,4-pentadiene (penta-1,4-diene)
c. 3-vinyl-1,4-cyclohexadiene (cyclohexa-1,4-diene)

Answer

a) 

b) 

c) 

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1. Vollhardt, Peter, and Neil E. Schore. Organic Chemistry: Structure and Function. 5th Edition. New York: W. H. Freeman & Company, 2007.