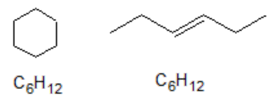
3.6: ALKENES

learning objectives

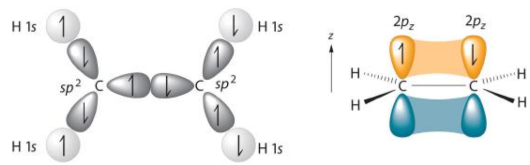
- name alkenes using IUPAC (systematic) and selected common name nomenclature
- draw the structure of alkenes from IUPAC (systematic) and selected common names

Alkenes contain carbon-carbon double bonds and are unsaturated hydrocarbons with the molecular formula is C_nH_{2n}. Be aware - this is also the same molecular formula ratio as cycloalkanes as shown in the example below.



INTRODUCTION

The parent structure is the longest chain containing both carbon atoms of the double bond. The two carbon atoms of a double bond and the four atoms attached to them lie in a plane, with bond angles of approximately 120° A double bond consists of one sigma bond formed by overlap of sp^2 hybrid orbitals and one pi bond formed by overlap of parallel 2 p orbitals.



(a) C_2H_4 σ-bonded framework **(b) C_2H_4 π bonding**

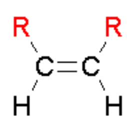
The carbon atoms sharing the double bond can be referred to as the "vinyl carbons". This common name arose because alkenes the source for vinyl polymers.

PI BOND RIGIDITY & GEOMETRIC ISOMERS

The rigidity of the pi bond in alkenes creates the possibility of stereoisomers called geometric isomers. To name alkenes, it may be neccessary to communicate the stereochemistry of the structure using the cis/trans or E/Z systems.

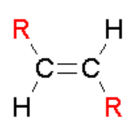
CIS ISOMERS

The two largest groups are on the same side of the double bond.



TRANS ISOMERS

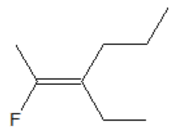
The two largest groups are on opposite sides of the double bond.



E/Z NOMENCLATURE

When the cis/trans system is ambiguous, the E/Z system can be used where E = entgegan ("trans") and Z = zusamen ("cis"). The E/Z system is used to prioritize when there are 3 or 4 different non-hydrogen atoms are attached to the vinyl carbons (carbons sharing the double bond). This system bases priority on the atomic number (Z) and/or atomic mass (A) of the atoms bonded to the vinyl carbons. An atom attached by a multiple bond is counted once for each bond. If there is a tie in priority, then move to the next atom along each chain until a difference occurs. Atomic number has higher priority than atomic mass. Atomic mass is used to establish priority for isotopes, therefore deuterium (D) has higher priority than hydrogen (H).

For example, when comparing atoms bonded to the vinylic carbons in the the compound below,



we would rank the priority as

fluorine atom > propyl group > ethyl group > methyl

Z = 9 > 3 x C chain > 2 x C chain > 1 x C chain

and name the compound ((2E)-3-ethyl-2-fluorohex-2-ene.

The double bond of the allylic group creates higher priority over a simple propyl grup such that $-CH_2-CH=CH_2 > -CH_2CH_2CH_3$.

For straight chain alkenes, it is the same basic rules as nomenclature of alkanes except change the suffix to "-ene."

1. Find the Longest Carbon Chain that Contains the Carbon Carbon double bond. If you have two ties for longest Carbon chain, and both chains contain a Carbon Carbon double bond, then identify the most substituted chain.

2. Give the lowest possible number to the Carbon Carbon double bond.

a) Do not need to number cycloalkenes because it is understood that the double bond is in the one position.

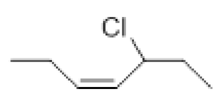
b) Alkenes that have the same molecular formula but the location of the double bonds are different means they are constitutional isomers.

c) Functional Groups with higher priority determine the suffix

3. Add substituents and their position to the alkene as prefixes. Of course remember to give the lowest numbers possible. And remember to name them in alphabetical order when writting them.

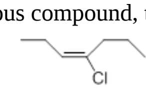
4. Next is identifying stereoisomers - cis/trans. when there are only two non hydrogen attachments to the alkene then use cis and trans to name the molecule.

For example, the compound below is a cis isomer. It has both the substituents going upward. This molecule would be called (cis) 5-chloro-3-heptene.



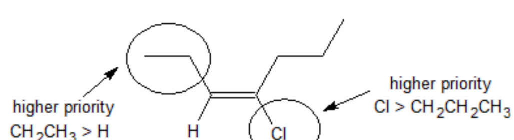
5. Next is identifying stereoisomers - E/Z if cis/trans is ambiguous or skip 4 above and jump straight to E/Z.

For example, if we look at the "trans" alternative lo the previous compound, the cis/trans system cannot be applied.



cis or trans?

This molecule would be called (3E)-4-chlorohept-3-ene. It is E because the ethyl group ($-CH_2CH_3$) has the higher priority for the vicinal carbon on the left and the chlorine atom has the higher priority for the vicinal carbon on the right and these two groups are on opposite sides of the double bond.



(3*E*)-4-chlorohept-3-ene

6. An example of functional group priorities in nomenclature is that the hydroxyl group gets precedence (has higher priority) over the double bond.

Therefore, alkenes containing alcohol groups are called alkenols with the sufffix --enol.

7. Lastly remember that alkene substituents are called alkenyl. Suffix --enyl.

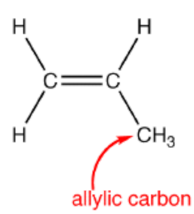
Here is a chart containing the systemic name for the first twenty straight chain alkenes.

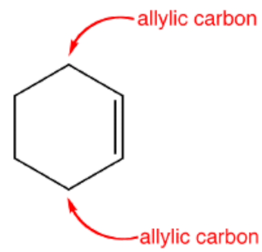
Name	Molecular formula
Ethene	C_2H_4
Propene	C_3H_6
Butene	C_4H_8
Pentene	C_5H_{10}
Hexene	C_6H_{12}
Heptene	C_7H_{14}
Octene	C_8H_{16}
Nonene	C_9H_{18}
Decene	$C_{10}H_{20}$
Undecene	$C_{11}H_{22}$
Dodecene	$C_{12}H_{24}$
Tridecene	$C_{13}H_{26}$
Tetradecene	$C_{14}H_{28}$
Pentadecene	$C_{15}H_{30}$
Hexadecene	$C_{16}H_{32}$
Heptadecene	$C_{17}H_{34}$
Octadecene	$C_{18}H_{36}$
Nonadecene	$C_{19}H_{38}$
Eicosene	$C_{20}H_{40}$

Did you notice how there is no methene? Because it is impossible for a carbon to have a double bond with nothing.

COMMON NAMES

The carbon atoms sharing the double bond can be referred to as the "vinyl carbons". The carbon atoms adjacent to the vinyl carbon atoms are called "allylic carbons". These carbon atoms have unique reactivity because of the potential for interaction with the pi bond.

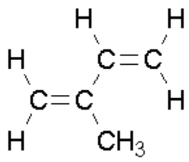




Overall, remove the -ane suffix and add -ylene.

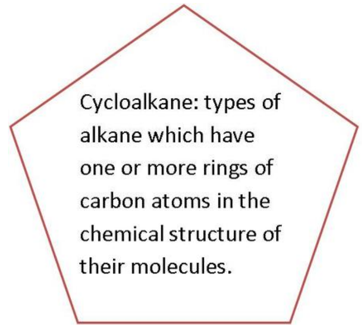
There are a couple of unique ones like ethenyl's common name is vinyl and 2-propenyl's common name is allyl, that you should know are...

- vinyl substituent H_2C=CH-
- allyl substituent H_2C=CH-CH_2-
- allene molecule H_2C=C=CH_2
- isoprene is shown below

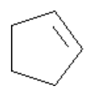


ENDOCYCLIC & EXOCYCLIC ALKENES

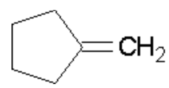
Endocyclic double bonds have both carbons in the ring and exocyclic double bonds have only one carbon as part of the ring.



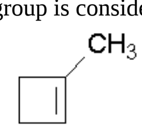
Cyclopentene is an example of an endocyclic double bond.



Methylenecylopentane is an example of an exocyclic double bond.

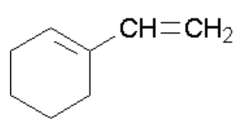


For example, when naming the compound below, the methyl group is considered when numbering the double bond.

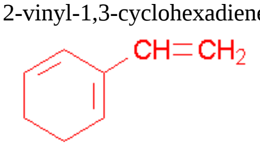


The compound can be named 1-methylcyclobutene or 1-methylcyclobut-1-ene.

When naming this next compound, the ethenyl group is considered when numbering the double bond.



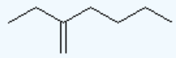
The IUPAC name for the compound can be 1-ethenylcyclohexene or 1-ethenylcyclohex-1-ene. The common name would be 1-vinylcyclohexene. For the compound below, the name is 2-vinyl-1,3-cyclohexadiene.

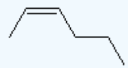


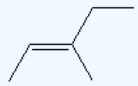
Exercise

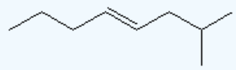
1. Give the IUPAC name for the following compounds. When stereochemistry is included, write the name using both the cis/trans and E/Z names if possible.

a) 

b) 

c) 

d) 

e) 

2. Draw the bond-line structures for the following compounds.

a) trans-2-pentene

b) (Z)-3-heptene

c) 4-methyl-2-pentene

d) (Z)-5-Chloro-3-ethly-4-hexen-2-ol.

Answer

1. a) 1-pentene or pent-1-ene

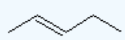
b) 2-ethyl-1-hexene or 2-ethylhex-1-ene (parent chain must include the double bond)

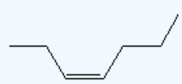
c) cis-2-hexene or (Z)-2-hexene or (2Z)-hex-2-ene

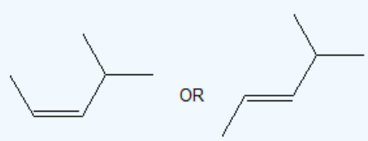
d) (2E)-3-methylpent-2-ene or (E)-3-methyl-2-pentene (cis/trans cannnt be applied)

e) trans-2-methyl-4-octene or (4E)-2-methyloct-4-ene or (E)-2-methyl-4-octene (branch breaks the tie in numbering the parent chain since both directions begin the double bond at carbon 4.

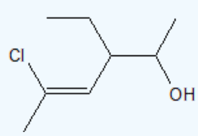
2.

a) 

b) 

c) 

no stereochemistry specified

d) 

OUTSIDE LINKS

- http://www.vanderbilt.edu/AnS/Chemis...0a/alkenes.pdf

REFERENCES

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

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