3.7: ALKYNES

learning objectives

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

Alkynes are organic molecules made of the functional group carbon-carbon triple bonds and are written in the empirical formula of \(C_nH_{2n-2}\). They are unsaturated hydrocarbons. Like alkenes have the suffix –ene, alkynes use the ending –yne; this suffix is used when there is only one alkyne in the molecule.

STRAIGHT CHAIN ALKYNES

Here are the molecular formulas and names of the first ten carbon straight chain alkynes.

Name	Molecular Formula
Ethyne	C_2H_2
Propyne	C_3H_4
1-Butyne	C_4H_6
1-Pentyne	C_5H_8
1-Hexyne	C_6H_{10}
1-Heptyne	C_7H_{12}
1-Octyne	C_8H_{14}
1-Nonyne	C_9H_{16}
1-Decyne	$C_{10}H_{18}$

NAMING ALKYNES

Like previously mentioned, the IUPAC rules are used for the naming of alkynes.

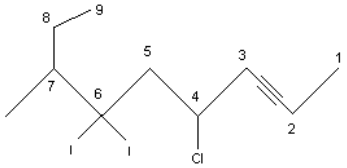
RULE 1

Find the longest carbon chain that includes both carbons of the triple bond.

RULE 2

Number the longest chain starting at the end closest to the triple bond. A 1-alkyne is referred to as a terminal alkyne and alkynes at any other position are called internal alkynes.

For example:

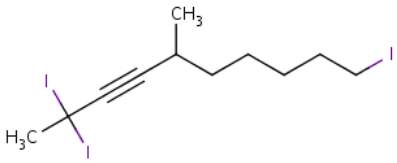


4-chloro-6-diiodo-7-methyl-2-nonyne

RULE 3

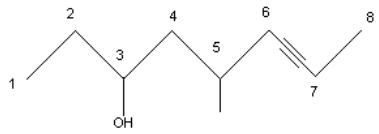
After numbering the longest chain with the lowest number assigned to the alkyne, label each of the substituents at its corresponding carbon. While writing out the name of the molecule, arrange the substituents in alphabetical order. If there are more than one of the same substituent use the prefixes di, tri, and tetra for two, three, and four substituents respectively. These prefixes are not taken into account in the alphabetical order.

For example:



1-triiodo-4-dimethyl-2-nonyne

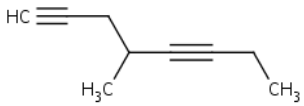
If there is an alcohol present in the molecule, number the longest chain starting at the end closest to it, and follow the same rules. However, the suffix would be –ynol, because the alcohol group takes priority over the triple bond.



5- methyl-7-octyn-3-ol

When there are two triple bonds in the molecule, find the longest carbon chain including both the triple bonds. Number the longest chain starting at the end closest to the triple bond that appears first. The suffix that would be used to name this molecule would be –diyne.

For example:

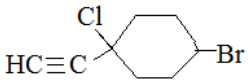


4-methyl-1,5-octadiyne

RULE 4

Substituents containing a triple bond are called alkynyl.

For example:



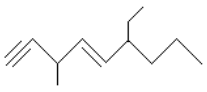
1-chloro-1-ethynyl-4-bromocyclohexane

Here is a table with a few of the alkynyl substituents:

Name	Molecule
Ethynyl	-C?CH
2- Propynyl	-CH_2C? CH
2-Butynyl	-CH_3C? CH_2CH_3

RULE 5

A molecule that contains both double and triple bonds is called an alkenyne. The chain can be numbered starting with the end closest to the functional group that appears first. For example:



6-ethyl-3-methyl-1,4-nonenyne

COMMON NAMES

The more commonly used name for ethyne is acetylene, which used industrially.

Similar to the allylic carbon position of alkenes, the carbons bonded to the alkyne carbons are called "propargyl" carbons and also have differences in chemical reactivity because of the interaction of the two pi bonds with the propargyl carbons.

HC≡CH–CH_2– Propargyl group

Exercise

1. Briefly identify the important differences between an alkene and an alkyne. How are they similar?

2. The alkene $(CH_3)_2CHCH_2CH=CH_2$ is named 4-methyl-1-pentene. What is the name of $(CH_3)_2CHCH_2C\equiv CH$?

3. Do alkynes show cis-trans isomerism? Explain.

4. Draw the bond-line structure & write the condensed structural formula for each compound except (a). For part (a) write the condensed formula and full Lewis (Kekule) structure.

a) acetylene

b) 3-octyne

c) 3-methyl-1-hexyne

d) 4,4-dimethyl-2-pentyne

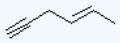
e) trans-3-hepten-1-yne

5. Give the IUPAC (Systematic) name for each compound.

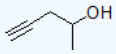
a) $CH_3CH_2CH_2C\equiv CH$

b) $CH_3CH_2CH_2C\equiv CCH_3$

c) 

d) 

e) 

f) 

Answer

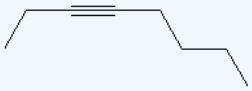
1. Alkenes have double bonds; alkynes have triple bonds. Both bonds are rigid and do not undergo rotation, however, the pi bonds allow both alkenes and alkynes to undergo addition reactions.

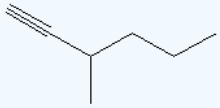
2. 4-methyl-1-pentyne

3. No; a triply bonded carbon atom can form only one other bond and has linear electron geometry so there are no "sides". Allkenes have two groups attached to each inyl carbon with a trigonal planar electron geometry that creates the possibility of cis-trans isomerism.

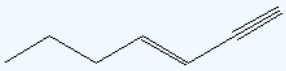
4.

a) CHCH

b)  $CH_3CH_2CCCH_2CH_2CH_2CH_3$

c)  $CHCCH(CH_3)CH_2CH_2CH_3$

d)  $CH_3CCC(CH_3)_3$

e)  $CH_3CH_2CH_2CHCHCCH$

5. a) 1-pentyne or pent-1-yne

b) 2-hexyne or hex-2-yne

c) 2-methylnon-4-yne or 2-methyl-4-nonyne

d) (4E)-hex-4-en-1-yne or (E)-hex-4-en-1-yne (alkynes have higher priority over alkenes if they occur sooner in the parent chain)

e) pent-1-en-4-yne (alkenes have higher priority over alkynes when they have the same position in the parent chain)

f) pent-4yn-2-ol (alcohols have higher priority than alkynes)

REFERENCE

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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