Hydrocarbon Isomers, Substituted Cycloalkanes and Aromatics

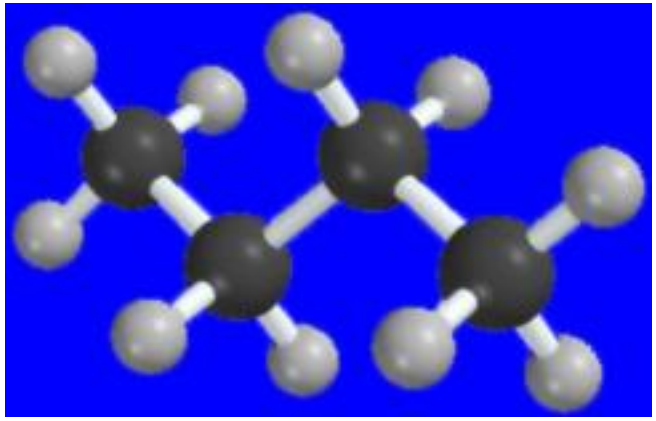
1) STRUCTURAL ISOMERS

-Same molecular formula but different structural formula
-Must have a different name

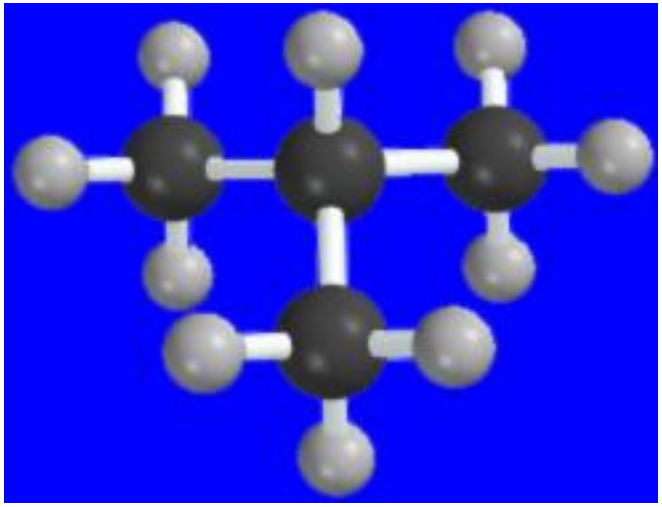
Isomeric Alkanes: The Butanes

C_4H_{10}

- Butane $CH_3CH_2CH_2CH_3$
- Methyl propane (Isobutane) $(CH_3)_3CH$



Butane
Bp: -0.4°C



Methyl propane
Bp: -10.2°C

Higher numbered Alkanes

$CH_3CH_2CH_2CH_2CH_3$

Pentane

$CH_3CH_2CH_2CH_2CH_2CH_3$

Hexane

$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$

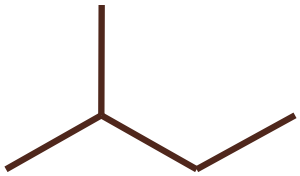
Heptane

The C_5H_{12} Isomers

C_5H_{12}

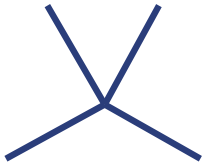
$CH_3CH_2CH_2CH_2CH_3$

Pentane



$(CH_3)_2CHCH_2CH_3$

2-methyl butane



$(CH_3)_4C$

Dimethyl propane

Draw and name the structural isomers for C_6H_{14}.

How many isomers?

The number of isomeric alkanes increases as the number of carbons increase.

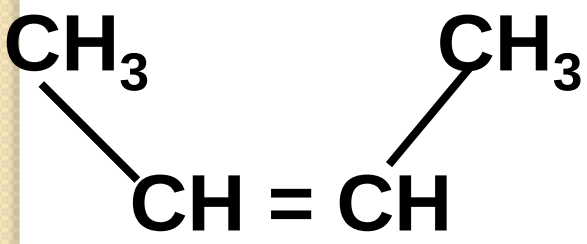
There is no simple way to predict how many isomers there are for a particular molecular formula.

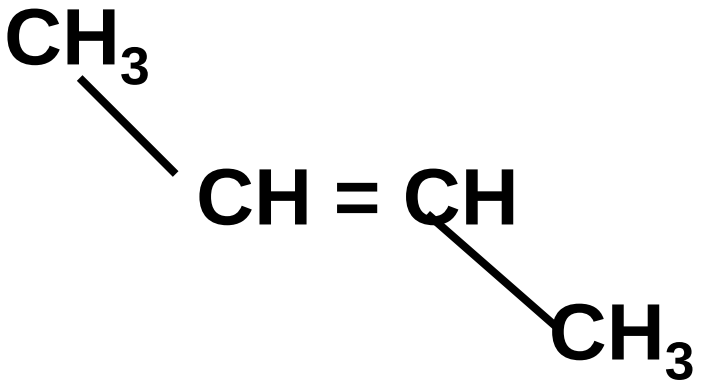
Number of Isomeric Alkanes

- CH_4 1
- C_2H_6 1
- C_3H_8 1
- C_4H_{10} 2
- C_5H_{12} 3
- C_6H_{14} 5
- C_7H_{16} 9
- C_8H_{18} 18
- C_9H_{20} 35
- $C_{10}H_{22}$ 75
- $C_{15}H_{32}$ 4,347
- $C_{20}H_{42}$ 366,319
- $C_{40}H_{82}$ 62,491,178,805,831

2) Geometric Isomers (Cis and Trans Isomers)

- Double bond is fixed; therefore this type only applies to alkenes
- Cis/trans Isomers are possible





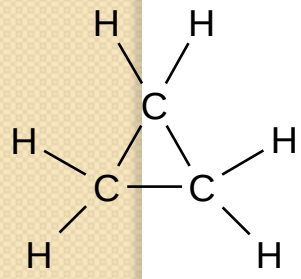
cis-2-butene

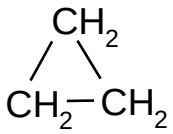
trans-2-butene

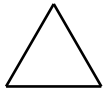
(SAME SIDE)

(ACROSS)

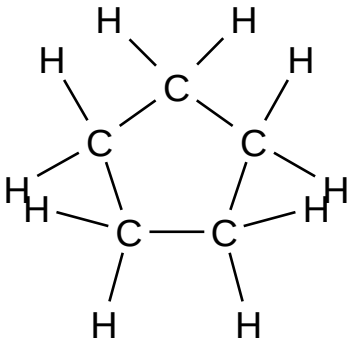
More on Cyclic Molecules/Cycloalkanes

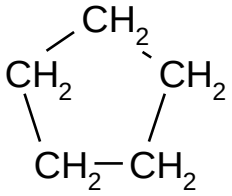


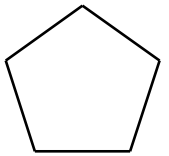




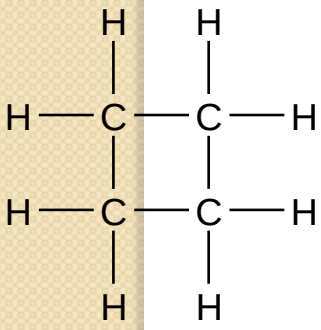
Cyclopropane

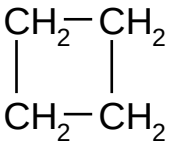


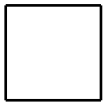




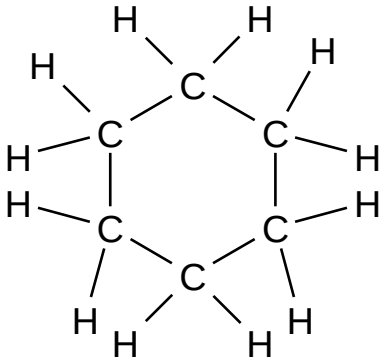
Cyclopentane

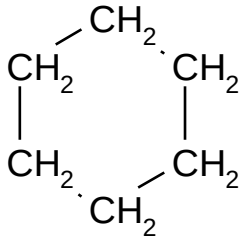


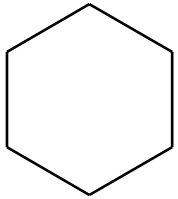




Cyclobutane



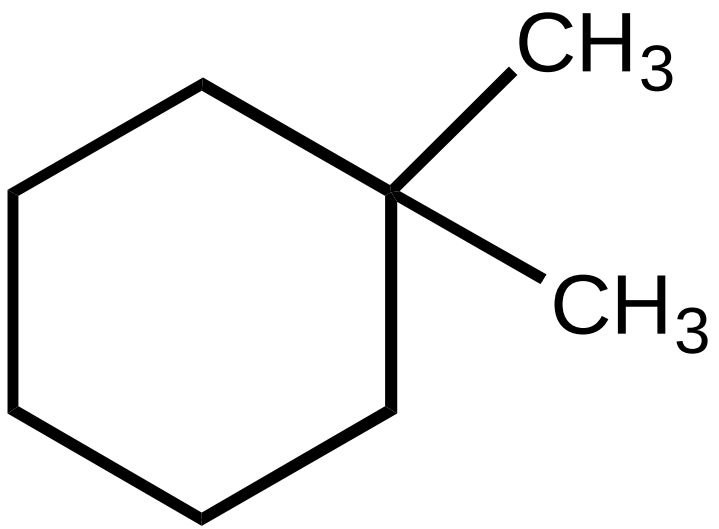




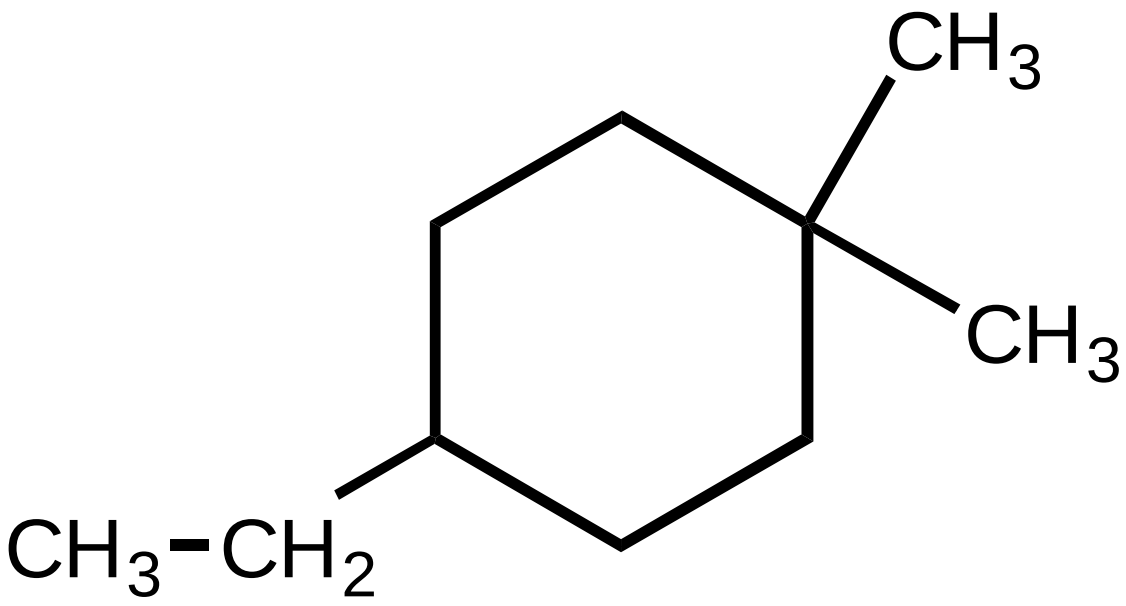
Cyclohexane

Nomenclature of the Substituted Cycloalkanes

- If there is only one branch, do not use the “1”.
- If there is more than one branch, you must use all numbers, including “1”!
- Number around the ring in either direction to get from the first branch to the second branch by the shorter path (the lowest numbers).
- If numbers are the same in either direction, start with the most complex branch.

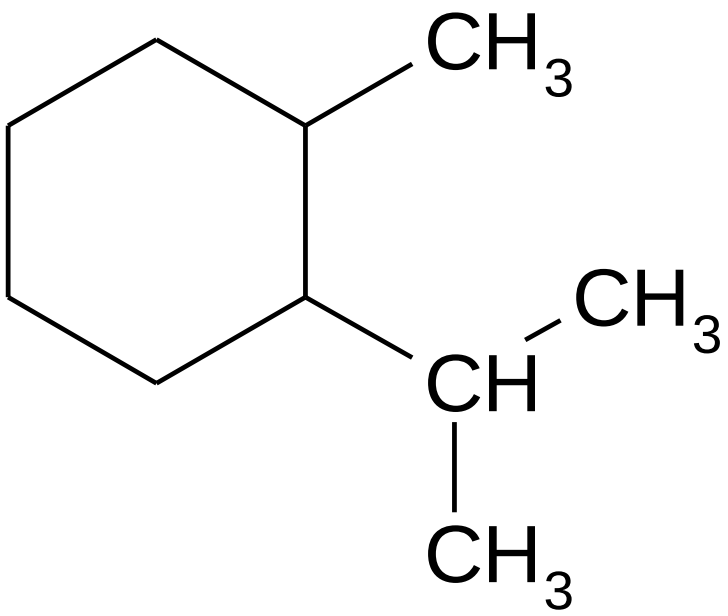


1,1-dimethylcyclohexane



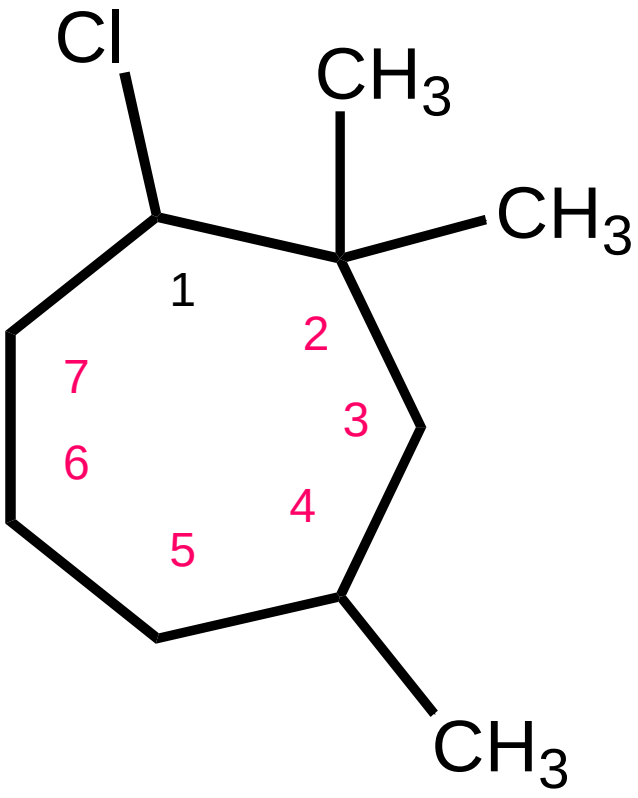
4-ethyl-1,1-dimethylcyclohexane

Since numbers are the same in either direction, start with the most complex branch.



1-isopropyl-2-methylcyclohexane

Number to achieve the lowest numbers for the branches.



1-chloro-2,2,4-trimethylcycloheptane

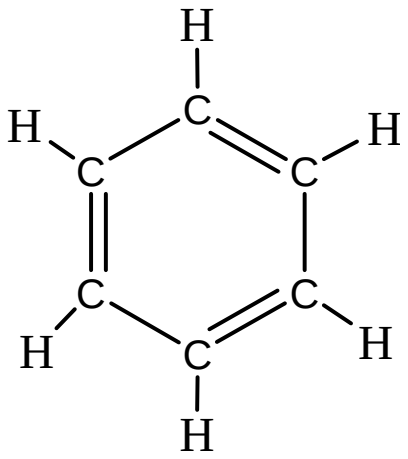
AROMATIC HYDROCARBONS

What are aromatic hydrocarbons?

- The term aromatic was first used to describe hydrocarbons with fragrant odours.
- However, now the term aromatic is used to describe the organic family which are derivatives of benzene
- Benzene is a very unique molecule that was first isolated from the oily residue that had collected in the gas lines in London, England

The Structure of Benzene

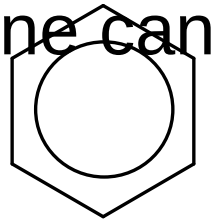
- Benzene has the molecular formula C_6H_6
- The structural formula of benzene consists of a 6-member carbon ring with 3 C=C double bonds



- The carbon-carbon bonds in benzene are all the same length which is evidence that the bonds are not true double and single bonds

If the bonds are not true single and double bonds what are they?

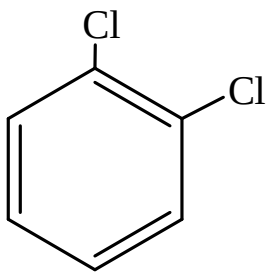
- The carbon-carbon bonds in benzene are all 139 pm which is intermediate between the length of a C-C single bond and a C=C double bond (double bonds are shorter).
- Therefore this indicates that the electrons that make up the “double bonds” in benzene are actually delocalized (i.e. shared) around all six carbon atoms equally.
- This arrangement of the electrons is indicated by placing a circle in the centre of the 6-member ring.
- Alternatively, benzene can be represented as below.



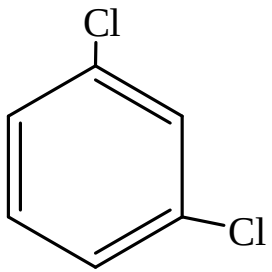
Naming Aromatics

1. Using benzene as the main chain:

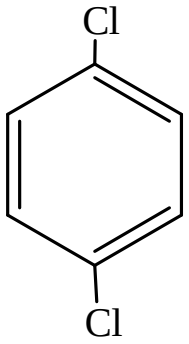
- Identify the groups attached and number accordingly.
- For compounds with 2 groups attached, the following prefixes may be used instead of the numbers;
- 1,2 = ortho 1,3 = meta 1,4 = para



ortho-dichlorobenzene



meta-dichlorobenzene



para-dichlorobenzene

2. When the benzene ring is not the main chain, phenyl is used to indicate a benzene ring as a branch.

Aromatic Practice

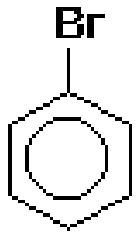
Draw the following:

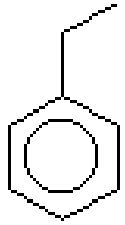
a) methylbenzene

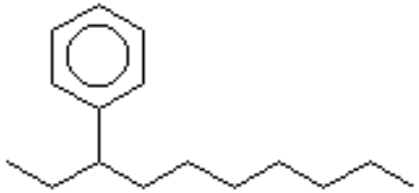
b) 1,3-diethyl-2-methylbenzene

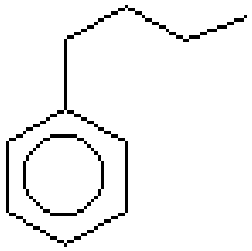
c) para-ethylpropylbenzene

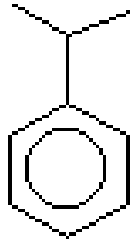
Name the following:



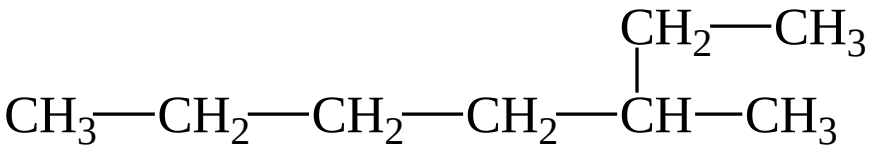




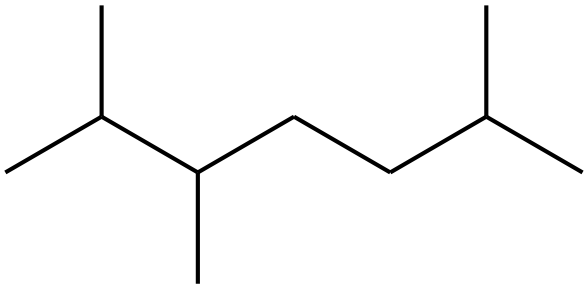




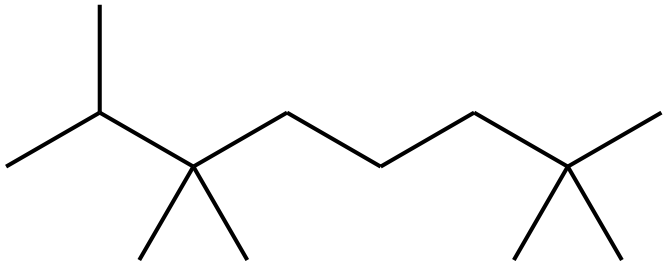
More Practice



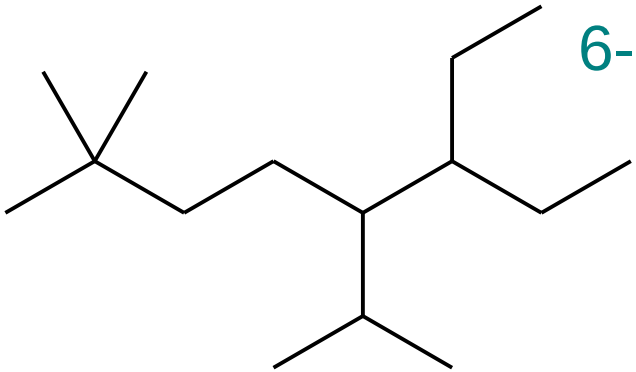
Longest chain is 7 (not 6).
This is 3-methylheptane.



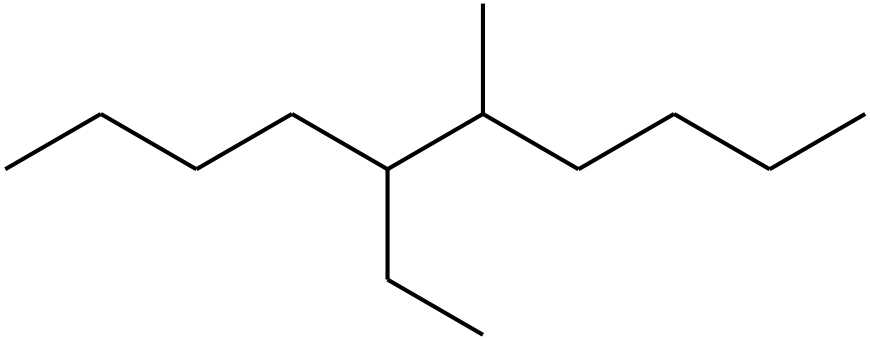
2,3,6-trimethylheptane.
(not 2,5,6-trimethyl heptane)



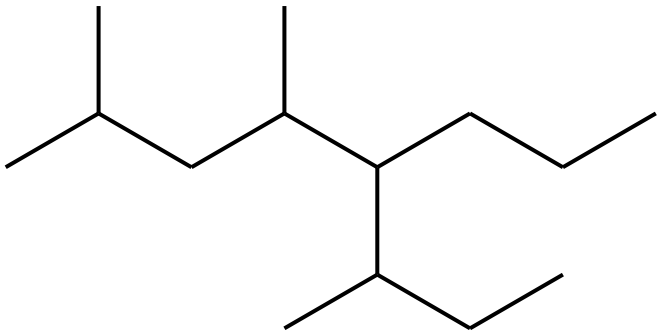
2,2,6,6,7-pentamethyloctane
or 2,3,3,7,7-pentamethyloctane??



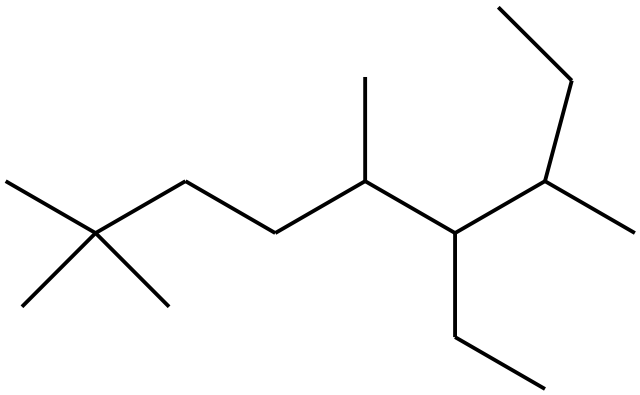
6-ethyl-5-isopropyl-2,2-dimethyloctane



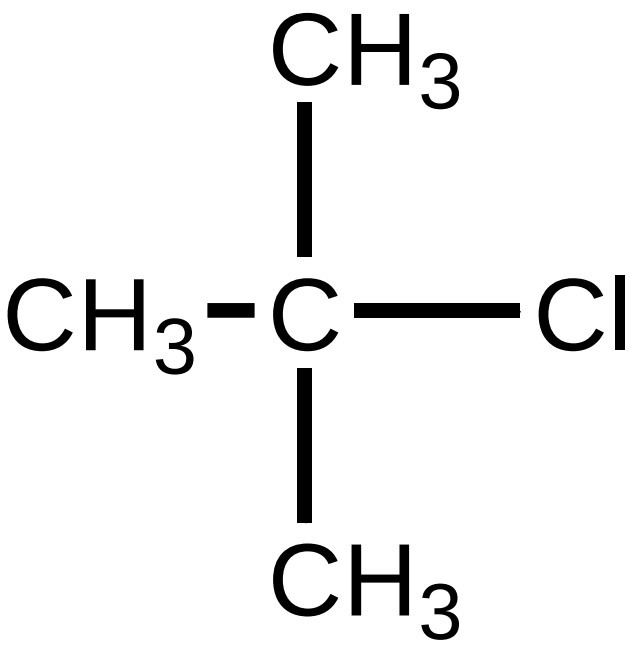
5-ethyl-6-methyldecane



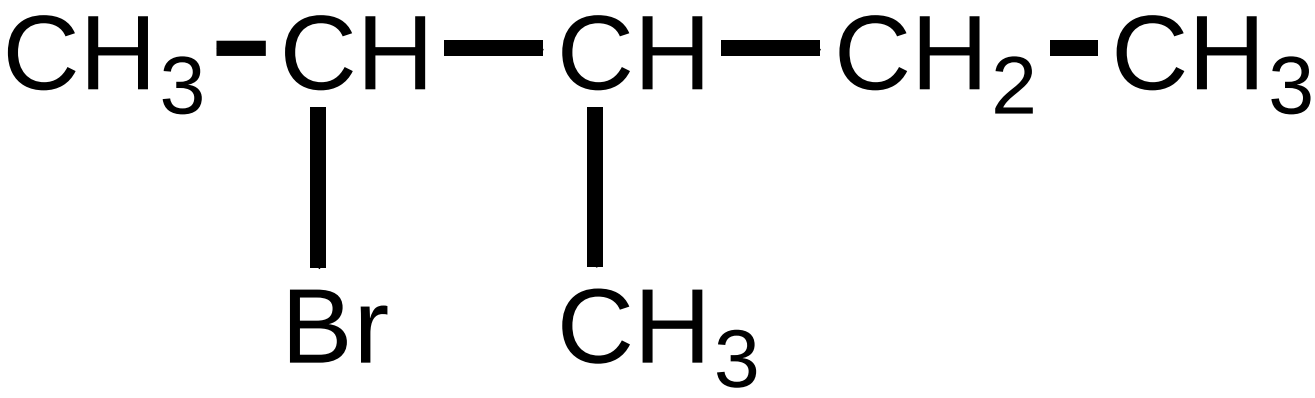
2,4,6-trimethyl-5-propyloctane



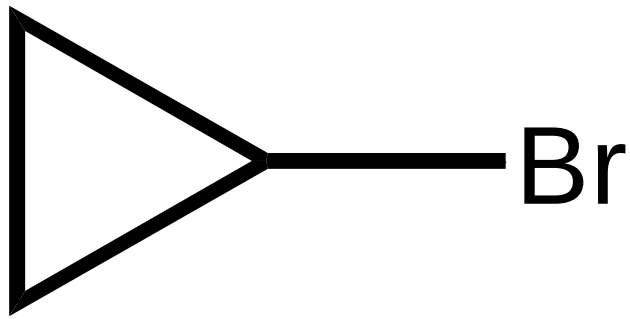
6-ethyl-2,2,5,7-
tetramethylnonane



2-chloro-2-methylpropane



2-Bromo-3-methylpentane



Bromocyclopropane

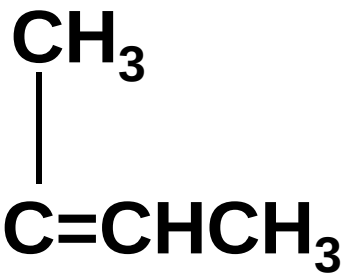
Learning Check

Write the IUPAC name for each of the following unsaturated compounds:

A. $CH_3CH_2C{\equiv}CCH_3$

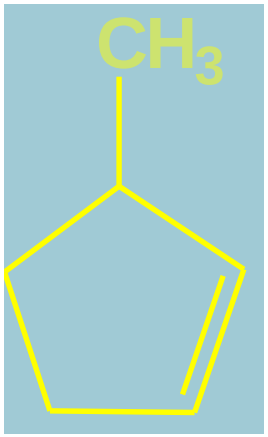
_____

B.



_____

C.



_____

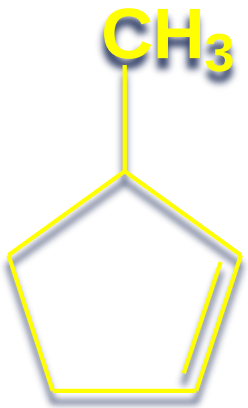
Solutions

Write the IUPAC name for each of the following unsaturated compounds:

A. $CH_3CH_2CH{=}CHCH_3$ **2-pentyne**

B. $CH_3C{=}CHCH_3$ **2-methyl-2-butene**

C.



3-methylcyclopentene