Isomerism

Isomers are molecules that have the same molecular formula but different structural formula

2 types:

1. Structural Isomers – atoms bonded in different orders

Isomerism – molecules with the same formula and different structures

2 Types

1) Structural Isomers

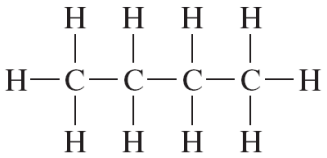
→ atoms bonded in different orders.

→ we will focus on alkanes (saturated hydrocarbons)

Structural Isomerism

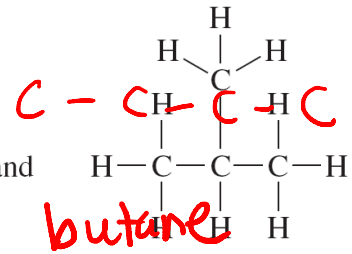
Ex. C_4H_{10}

C_4H_{10}

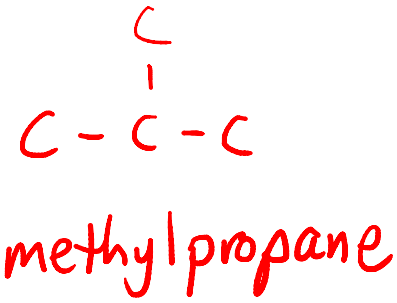


butane

and

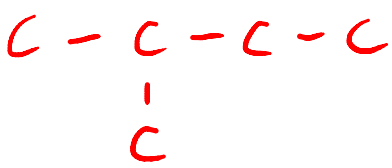


isobutane

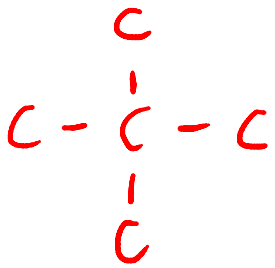


How many structural isomers for C_5H_{12}

pentane

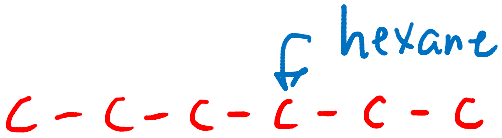


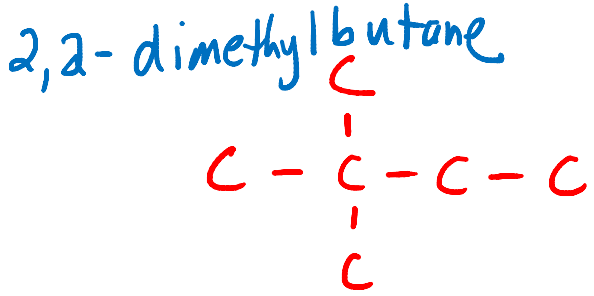
2-methylbutane

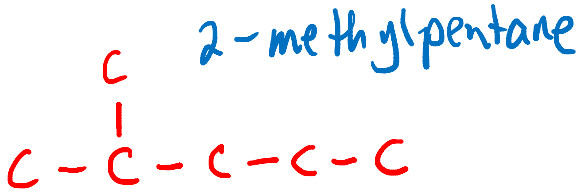


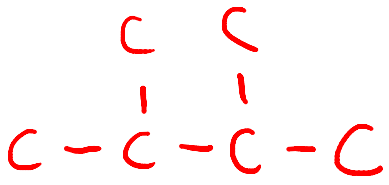
2,2-dimethylpropane

How many structural isomers for C_5H_{12}

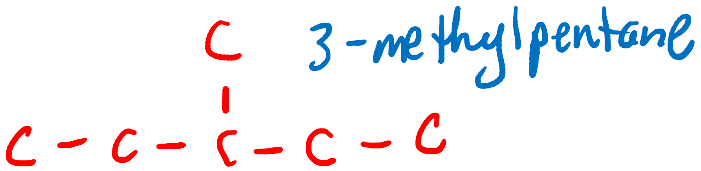








2,3-dimethyl butane



Geometric Isomerism

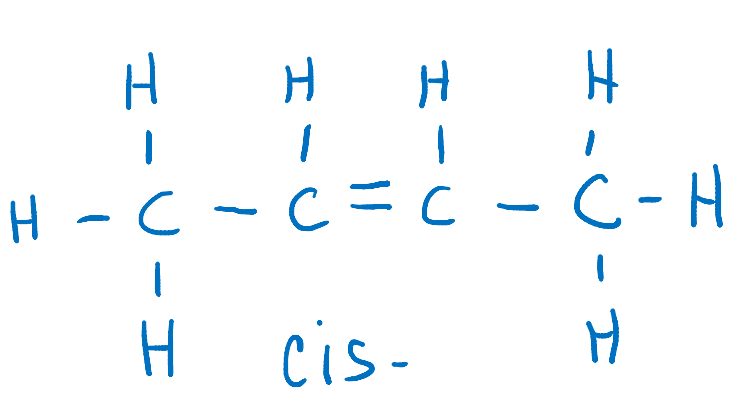
- 2. Geometric Isomers - atoms bonded in same order with different arrangement of atoms relative **to double bonded carbons**

2) Geometric Isomers

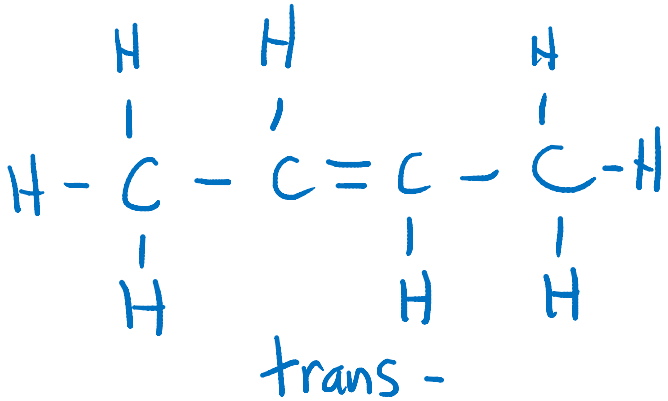
→ are found with alkenes

→ arrangement of atoms attached to double-bonded carbons.

inside (not on an end)

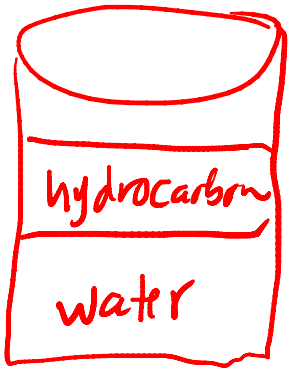


cis-



trans-

Properties of Hydrocarbons



1) Non-polar substances
2) Insoluble in water
3) Less dense than water
4) Very weak intermolecular forces
   → Van der Waals only (no polar bonds!)
5) Low melting points and low boiling points
6) Boiling points increase as carbons are added.
7) Undergo combustion reactions.

Combustion Reactions

hydrocarbon + O_2 $\longrightarrow$ CO_2 + H_2O

C_5H_{12} + O_2 $\longrightarrow$ CO_2 + H_2O

C_6H_{14} + O_2 $\longrightarrow$ CO_2 + H_2O

C_7H_{16} + O_2 $\longrightarrow$ CO_2 + H_2O

Balancing Tips -

balance C first

H second

O ALWAYS LAST.

$C_5H_{12} + 8O_2 \longrightarrow 5CO_2 + 6H_2O$

C - 5
H - 12
O - ~~2~~ 16

C - ~~1~~ 5
H - ~~2~~ 12
O - ~~3~~ ~~1~~ 16

$2C_6H_{14} + 19O_2 \longrightarrow 12CO_2 + 14H_2O$

24
14
38

C - 6
H - 14
O - ~~2~~ 38

C - ~~1~~ 6
H - ~~2~~ 14
O - ~~3~~ 13 ~~19~~ 38

uneven - double ALL

$C_7H_{16} + 11O_2 \longrightarrow 7CO_2 + 8H_2O$

14
8

C - 7
H - 16
O - ~~2~~ 22

C - ~~1~~ 7
H - ~~2~~ 16
O - ~~3~~ 15 22

Properties and uses of Alkanes

- See Table 20-5
- Carbon-hydrogen bonds are non-polar
- Hydrophobic; insoluble in water
- Less dense than water
- Forces of attraction simply dispersion forces (no H-bonding!!!)
- Strength of dispersion forces increases as mass increases

Saturated Hydrocarbons: Alkanes

Alkanes: Saturated – no double or triple bonds

General formula C_nH_{2n+2}

TABLE 19.3 | Names, Formulas, and Physical Properties of Straight-Chain Alkanes

Name	Molecular formula C_nH_{2n+2}	Condensed structural formula	Boiling point (°C)	Melting point (°C)
Methane	CH_4	CH_4	−161	−183
Ethane	C_2H_6	CH_3CH_3	−89	−172
Propane	C_3H_8	$CH_3CH_2CH_3$	−42	−187
Butane	C_4H_{10}	$CH_3CH_2CH_2CH_3$	−0.6	−135
Pentane	C_5H_{12}	$CH_3CH_2CH_2CH_2CH_3$	36	−130
Hexane	C_6H_{14}	$CH_3CH_2CH_2CH_2CH_2CH_3$	69	−95
Heptane	C_7H_{16}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$	98	−90
Octane	C_8H_{18}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	125	−57
Nonane	C_9H_{20}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	151	−54
Decane	$C_{10}H_{22}$	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	174	−30

- Combustion Reaction - type of chemical reaction that involves the combination of a hydrocarbon with oxygen to produce….
- H_2O, CO_2, and energy
- EX: $CH_4 + O_2 \text{ ----> } CO_2 + H_2O$ + energy
- - this is an exothermic reaction (energy is released)

Properties and uses of Alkanes

- Physical States
- Less than 4 carbons – gas
  - Natural gas – fossil fuel composed of primarily alkanes containing 1-4 carbons
- Larger alkanes – liquids (ex. Gasoline, kerosene)
- Very large alkanes – solids (ex. Paraffin wax)
- Note: strength of dispersion forces increases as mass increases

Properties and uses of Alkanes

- Boiling Points
- Increase with mass (dispersion forces)
- As mass increases, more heat needed to separate molecules
- Petroleum – complex mixture of different hydrocarbons that varies greatly in composition (1 to 50 carbons)
- This range allows separation through fractional distillation on the basis of different boiling points

Properties and uses of Alkanes

- Combustion – reaction that alkanes undergo which releases much energy
- Ex. $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O + 890\ kJ$
- Concern: release of greenhouse gases which may cause global warming
- Octane rating – measure of fuel burning efficiency and its antiknock properties
- When fuel ignites spontaneously, knocking results
- Straight chain alkanes more likely to knock
- Increasing branched chains in gas increases octane rating

Naming Organic Compounds

How do chemists name organic compounds?

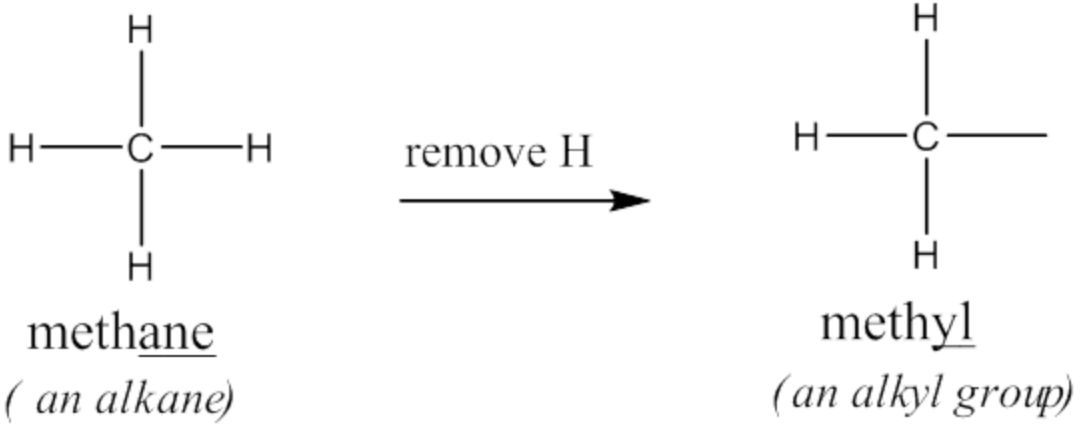
Organic compounds are named using the IUPAC System *(International Union of Pure and Applied Chemistry).*

The IUPAC System was developed at an international science meeting in Geneva in 1892.

The IUPAC System is essentially a set of rules that allow for a systematic and uniform method of naming compounds.

Alkyl Groups

Derived from alkane compounds
One hydrogen removed from a carbon
Open bond attaches to a parent chain
Alkyl name is derived from alkane name
    "ane" changed to "yl"
    i.e. methane becomes methyl



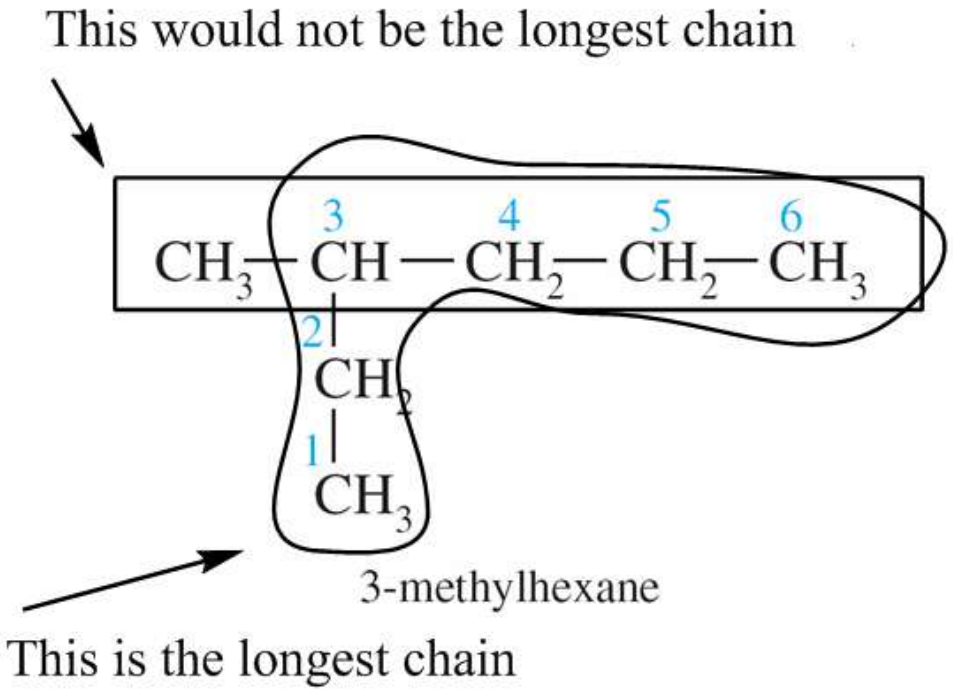
Naming Alkyl Groups

TABLE 19.4 | Names and Formulas of Selected Alkyl Groups

Formula	Name	Formula	Name
CH_3-	methyl	$CH_3CH(CH_3)-$	isopropyl
CH_3CH_2-	ethyl	$CH_3CH(CH_3)CH_2-$	isobutyl
$CH_3CH_2CH_2-$	propyl	$CH_3CH_2CH(CH_3)-$	*sec*-butyl (secondary butyl)
$CH_3CH_2CH_2CH_2-$	butyl	$CH_3C(CH_3)_2-$	*tert*-butyl or *t*-butyl (tertiary butyl)
$CH_3(CH_2)_3CH_2-$	pentyl		
$CH_3(CH_2)_4CH_2-$	hexyl		
$CH_3(CH_2)_5CH_2-$	heptyl		
$CH_3(CH_2)_6CH_2-$	octyl		
$CH_3(CH_2)_7CH_2-$	nonyl		
$CH_3(CH_2)_8CH_2-$	decyl		

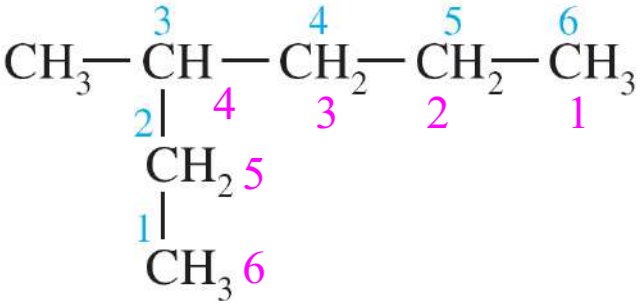
IUPAC Rules for Naming Alkanes

1. Identify and then name the longest continuous chain of carbon atoms. The longest chain in this molecule contains six carbon atoms.



IUPAC Rules for Naming Alkanes

2. Number the chain so any branch alkyl groups have the lowest possible number. There is only one correct way to number the carbon atoms in the longest chain.

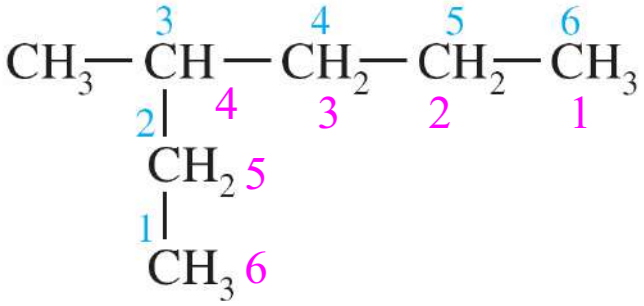


3-methylhexane

Numbering in this direction is incorrect because it gives the methyl branch a higher number, i.e. a 4 instead of a 3.

IUPAC Rules for Naming Alkanes

3. The methyl group is attached to the #3 carbon atom not the #4 carbon atom. The IUPAC name for the molecule is 3-methylhexane.

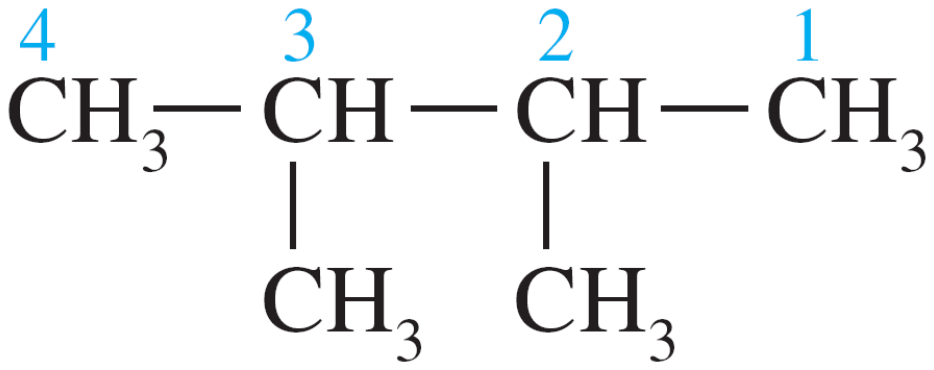


3-methylhexane

Numbering in this direction is incorrect because it gives the methyl branch a higher number, i.e. a 4 instead of a 3.

IUPAC Rules for Naming Alkanes

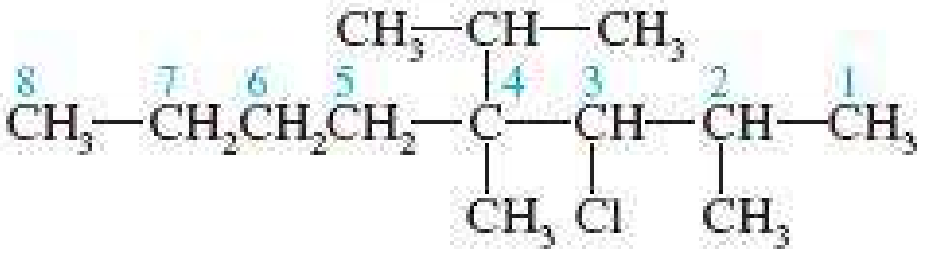
4. Use prefixes *(i.e. di, tri, tetra etc.)* if two or more of the same alkyl group branches appear on the longest chain. One methyl group is on the #2 carbon atom and another methyl group is on the #3 carbon atom.



2,3-dimethylbutane

IUPAC Rules for Naming Alkanes

5. When several different groups are attached to the same parent compound, list the groups in alphabetical order (e.g. chloro is listed before isopropyl and isopropyl is listed before methyl).



3-chloro-4-isopropyl-2,4-dimethyloctane

Examples

- Sample Problem 20-1, pg 639
-

- Sample Problem 20-2, pg 640
  - Draw the condensed structural formula of 3-ethyl-4-methylhexane

- Draw the structural formula of methylbutane.

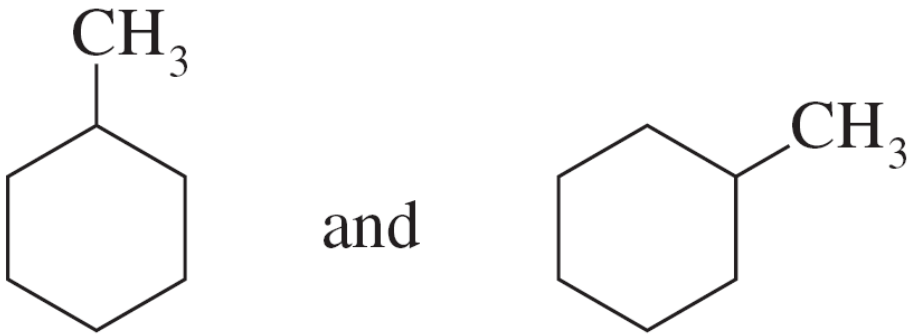
- Draw the structural formula for 3,3-diethyl-2,5-dimethylnonane

- Draw the structural formulas for the two structural isomers of methylpentane and name the isomers.

Cycloalkanes

When naming monosubstituted cycloalkanes:

1. Name the substituent
2. Name the parent cyclohexane



Both of these structures are the same molecule and have the same name (methylcyclohexane).

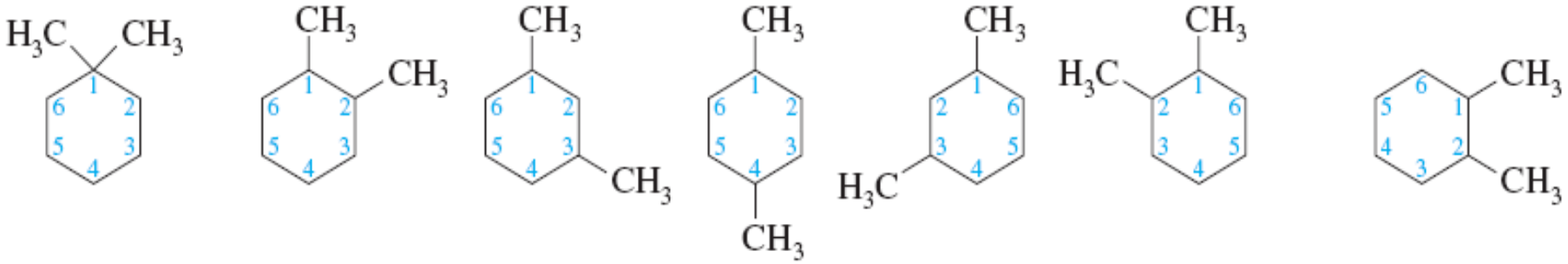
methyl + cyclohexane = methylcyclohexane

Cycloalkanes

When naming polysubstituted cycloalkanes.

1. Number the ring (clockwise or counterclockwise) to give the substituted groups the lowest possible numbers.
2. Name the groups and their locations.
3. Name the parent cyclohexane.

Cycloalkanes



A B C D E F G

A is 1,1-dimethylcyclohexane
B is 1,2-dimethylcyclohexane
C is 1,3-dimethylcyclohexane
D is 1,4-dimethylcyclohexane

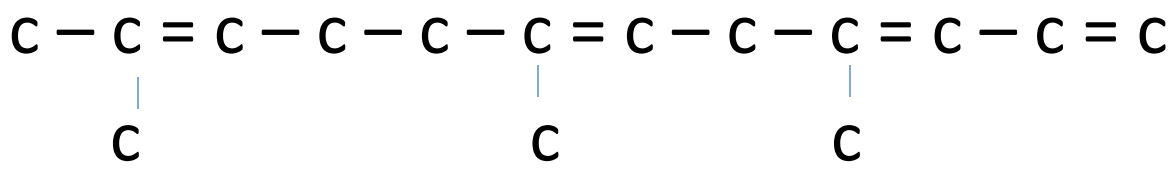
E is 1,3-dimethylcyclohexane (numbered counterclockwise)
F is 1,2-dimethylcyclohexane (numbered counterclockwise)
G is 1,2-dimethylcyclohexane (same as B and F)

Homework

- Pg 658 – 659 #s 34-37

Unsaturated Hydrocarbons

- Alkenes – at least one double bond
- Ex. Propane vs propene
- Cis and trans isomerism occur with alkenes
- <u>Properties</u>
  - Nonpolar and show trends in properties similar to alkanes
  - Farnesene (natural wax covering in apples)



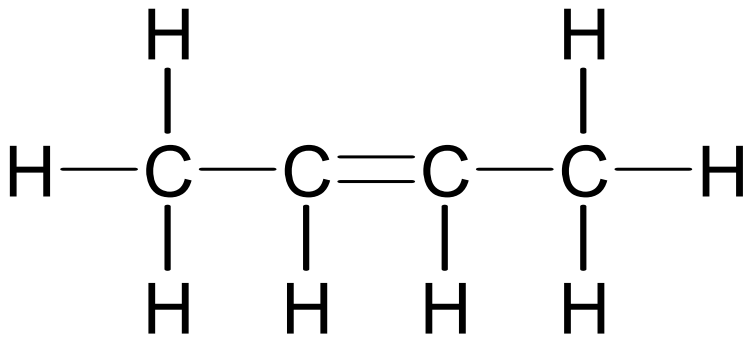
-ethene is a gas

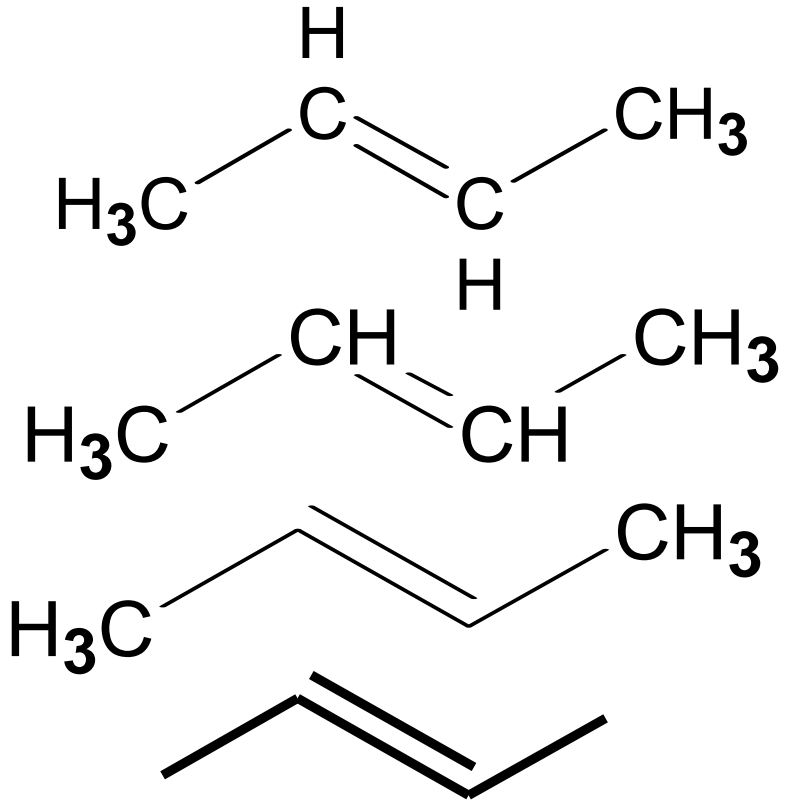
- Alkynes – contain at least one triple bond
- Ex. Propane vs propyne
- Similar properties to alkanes and alkenes
- Ethyne is a gas with the common name of acetylene (used in welding torches)

Naming Hydrocarbons
(nomenclature)

Drawing Structures: It's All Good

2-butene





$H_3C-CH=CH-CH_3$

This is called the "condensed structure"

$CH_3CH=CHCH_3$

On a test, choose a method that shows all Hs

Using brackets can also shorten some formulas:

$CH_3CH_2CH_2CH_2CH_2CH_3$ vs. $CH_3(CH_2)_4CH_3$

Basic Naming of Hydrocarbons

Hydrocarbon names are based on: 1) type, 2) # of carbons, 3) side chain type and position

1) name will end in -ane, -ene, or -yne

2) the number of carbons is given by a "prefix"

1 meth- 2 eth- 3 prop- 4 but- 5 pent- 6 hex- 7 hept- 8 oct- 9 non- 10 dec-

Actually, all end in a, but a is dropped when next to a vowel. E.g. a 6 C alkene is hexene

Q - What names would be given to these:

7C, 9C alkane heptane, nonane

2C, 4C alkyne ethyne, butyne

1C, 3C alkene ~~methene~~, propene

Mnemonic for First Four Prefixes

First four prefixes

- Meth- Monkeys
- Eth- Eat
- Prop- Peeled
- But- Bananas

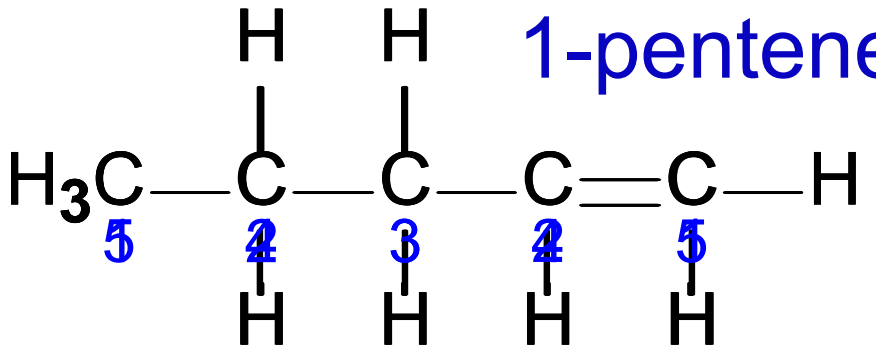
Other Prefixes

- Pent-
- Oct-
- Dec-
- Hex-, Hept-, Non-

Numbering Carbons

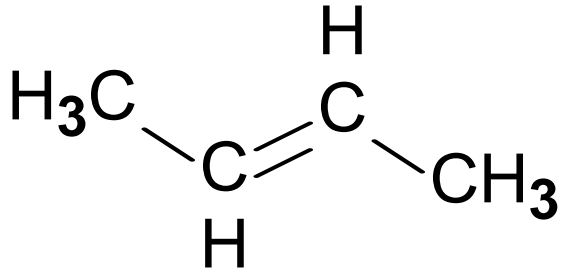
Q- draw pentene

A- Where's the double bond? We # C atoms.



1-pentene

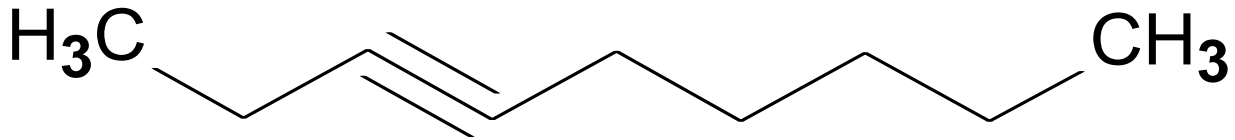
- Naming compounds with multiple bonds is more complex than previously indicated.
- When 2+ possibilities exist, #s are needed.
- Always give double bond the lowest number.
- Q - Name these



2-butene

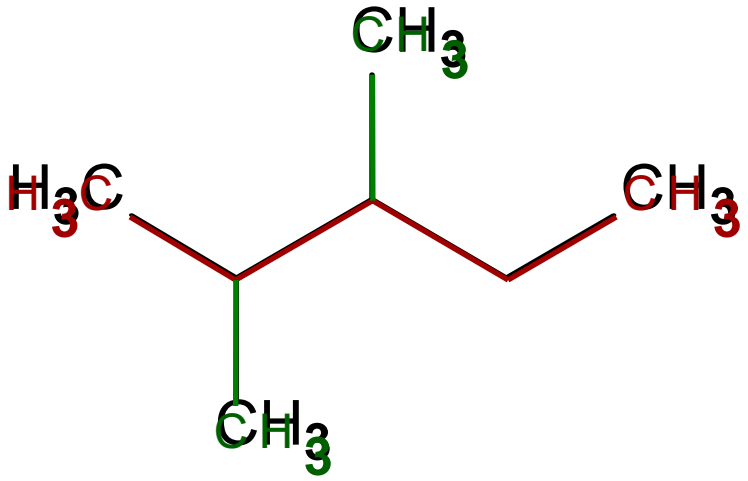
C_2H_4

ethene



3-nonyne

Naming Side Chains



- The names of molecules with branches are based on: side chains, root

  2,3-dimethylpentane

- The “root” or “parent chain” is usually the longest possible hydrocarbon chain.
- The root must include multiple bonds if they are present. If a cyclic structure is present it will be the root even if it is not the longest chain.
- Side chains are also called “side branches” or “alkyl groups”. Their names end in -yl.

<u>Common side chains</u> :

-CH_3 methyl, -CH_2CH_3 ethyl, -$CH_2CH_2CH_3$ propyl

IUPAC Rules for Naming Hydrocarbons

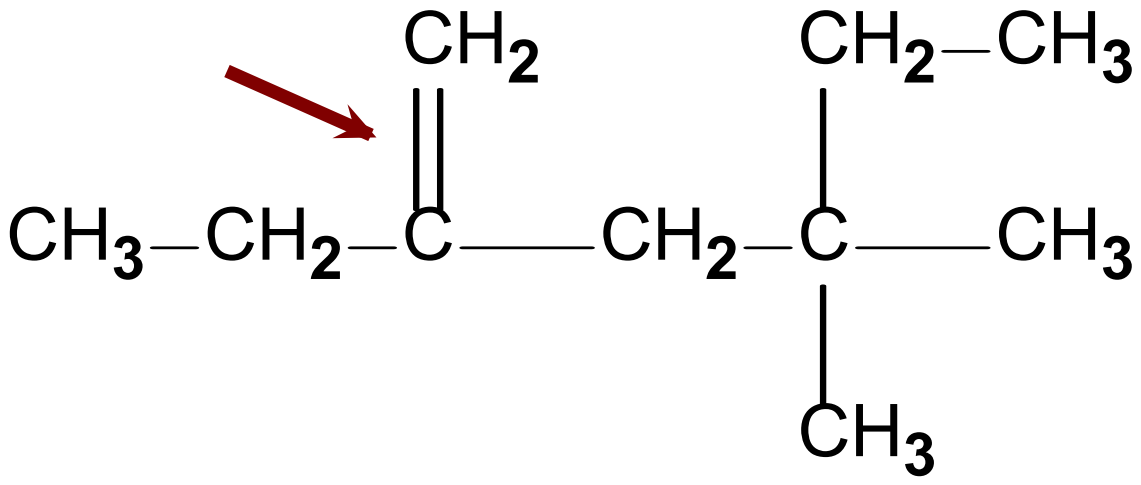
1. Choose the correct ending: -ane, -ene, or -yne
2. Determine the longest carbon chain. Where a double or triple bond is present, choose the longest chain that includes this bond. If there is a cyclic structure present, the longest chain starts and stops within the cyclic structure.
3. Assign numbers to each C of the parent chain. For alkenes and alkynes the first carbon of the multiple bond should have the smallest number. For alkanes the first branch (or first point of difference) should have the lowest #. Carbons in a multiple bond must be numbered consecutively.
4. Attach a prefix that corresponds to the number of carbons in the parent chain. Add cyclo- to the prefix if it is a cyclic structure.

IUPAC Rules for Naming Hydrocarbons

5. Determine the correct name for each branch ("alkyl" groups include methyl, ethyl, propyl, etc.)
6. Attach the name of the branches alphabetically, along with their carbon position, to the front of the parent chain name. Separate numbers from letters with hyphens (e.g. 4-ethyl-2-methyldecane)
7. When two or more branches are identical, use prefixes (di-, tri-, etc.) (e.g. 2,4-dimethylhexane). Numbers are separated with commas. Prefixes are ignored when determining alphabetical order. (e.g. 2,3,5-trimethyl-4-propylheptane)
8. When identical groups are on the same carbon, repeat the number of this carbon in the name. (e.g. 2,2-dimethylhexane)

Naming Side Chains

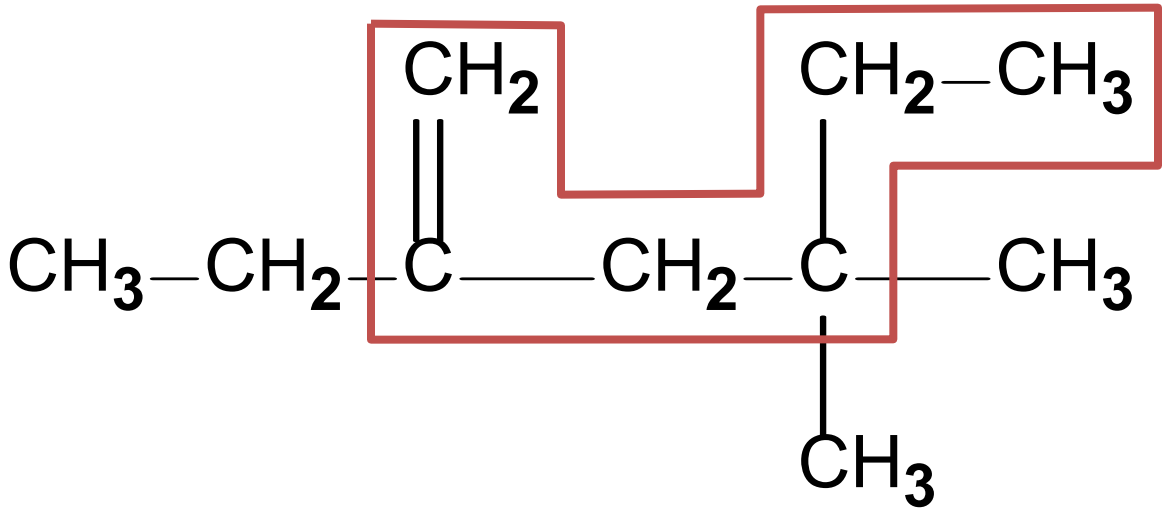
Example: use the rules on this handout to name the following structure



Rule 1: choose the correct ending

ene

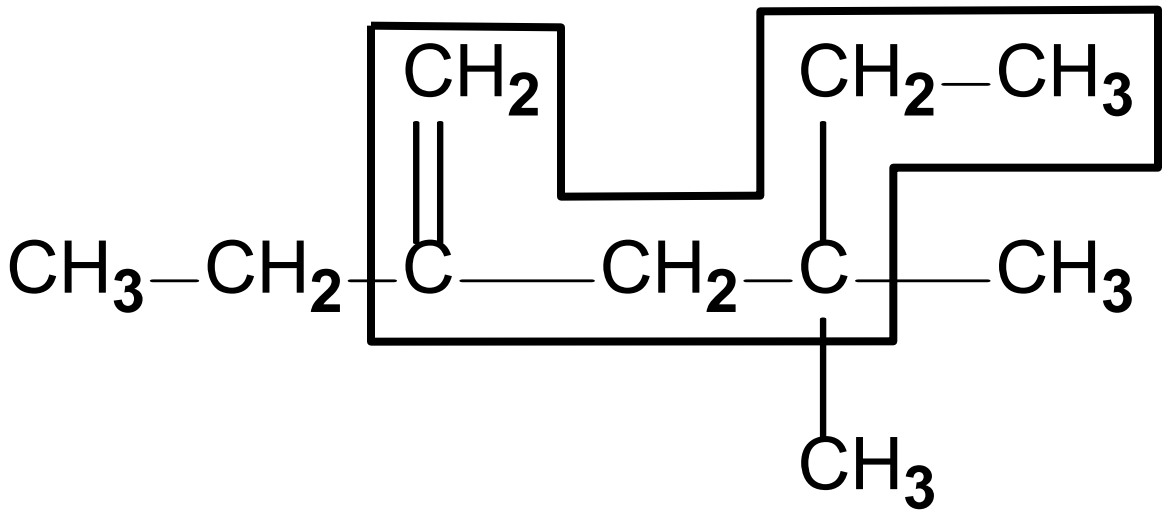
Naming Side Chains



Rule 2: determine the longest carbon chain

ene

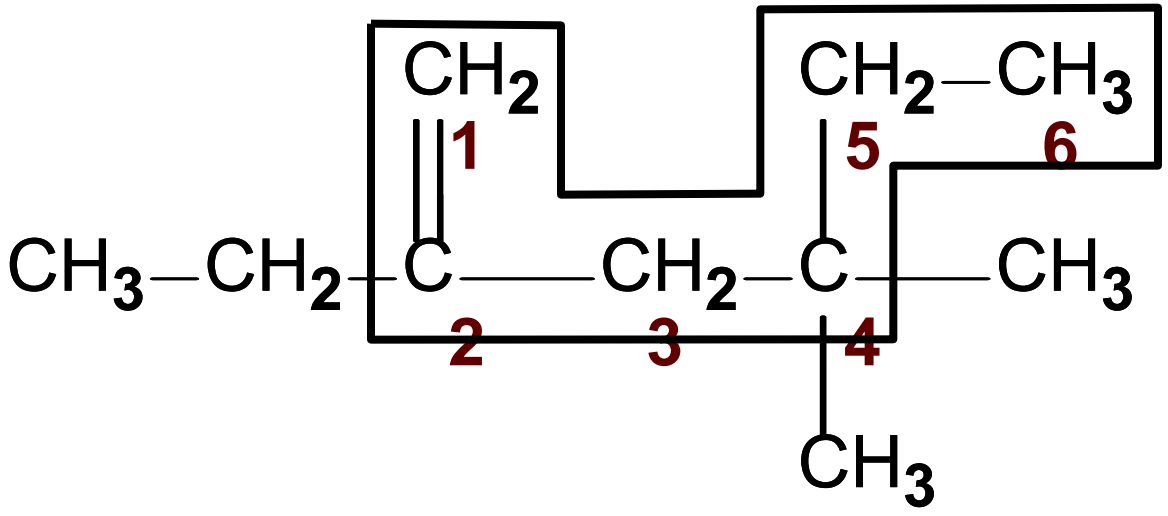
Naming Side Chains



Rule 3: Assign numbers to each carbon

ene

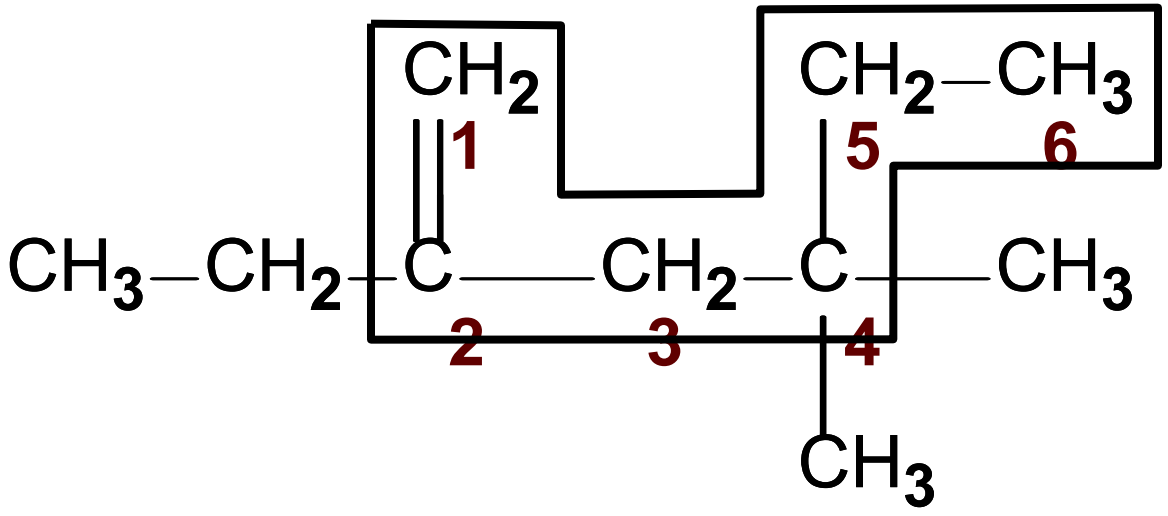
Naming Side Chains



Rule 3: Assign numbers to each carbon

ene

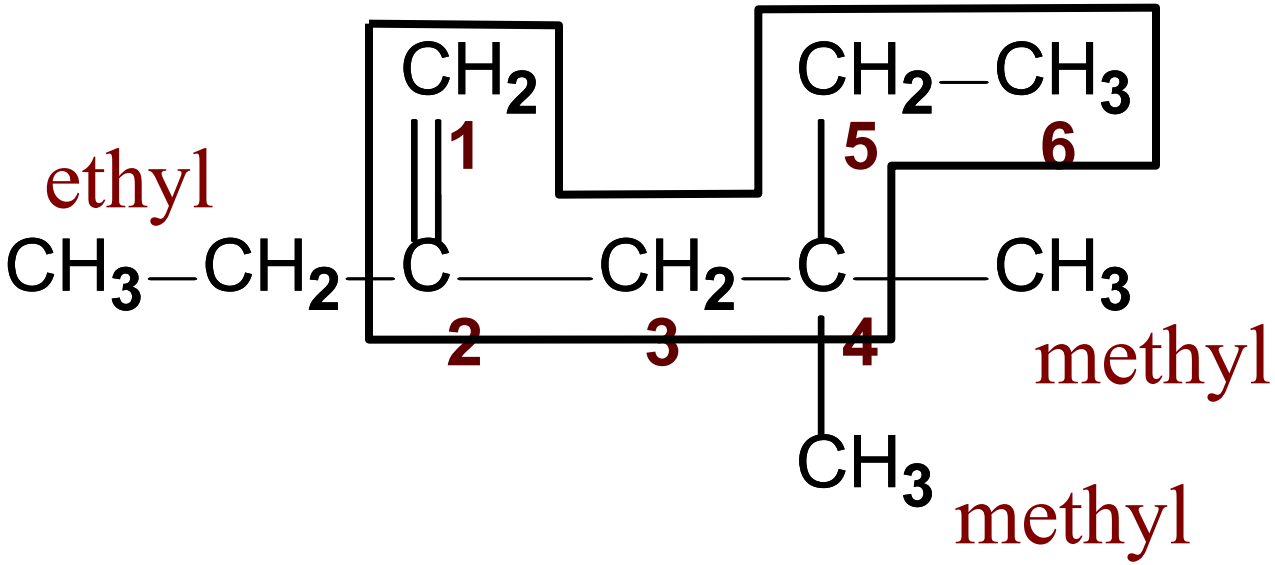
Naming Side Chains



Rule 4: attach prefix (according to # of Cs)

1-hexene

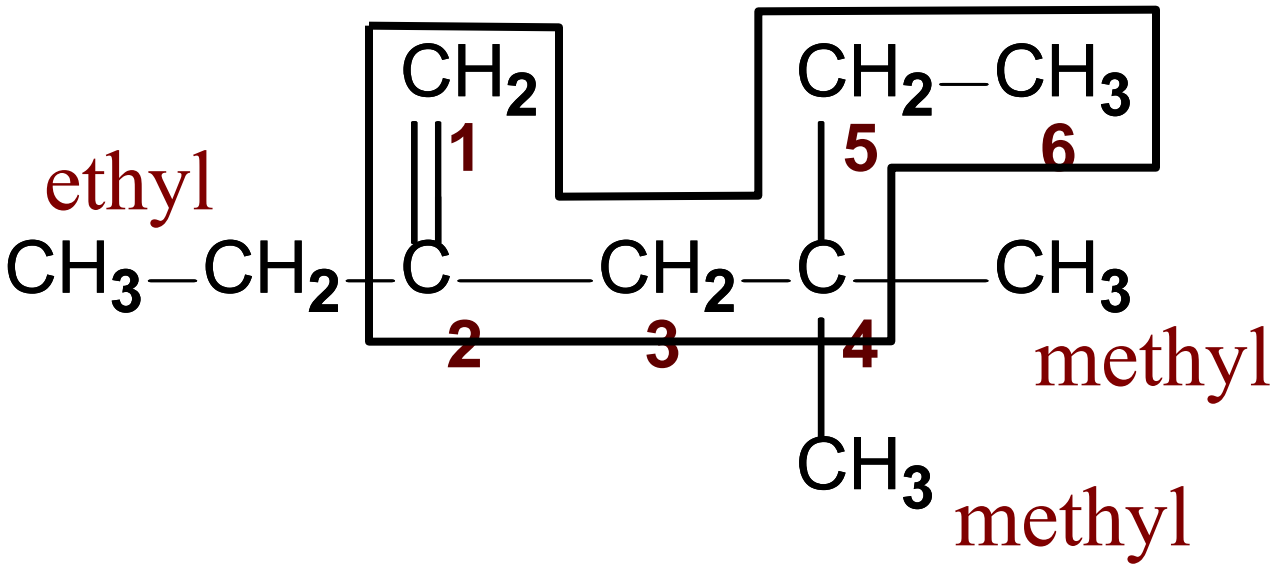
Naming Side Chains



Rule 5: Determine name for side chains

1-hexene

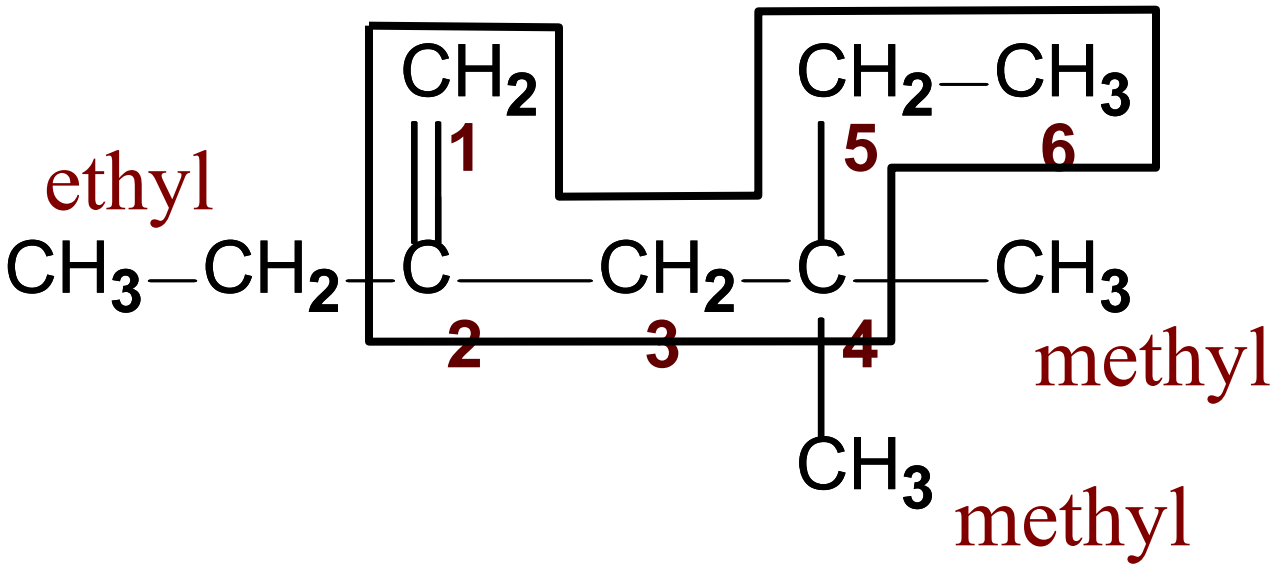
Naming Side Chains



Rule 6: attach name of branches alphabetically

2-ethyl-4-methyl-4-methyl-1-hexene

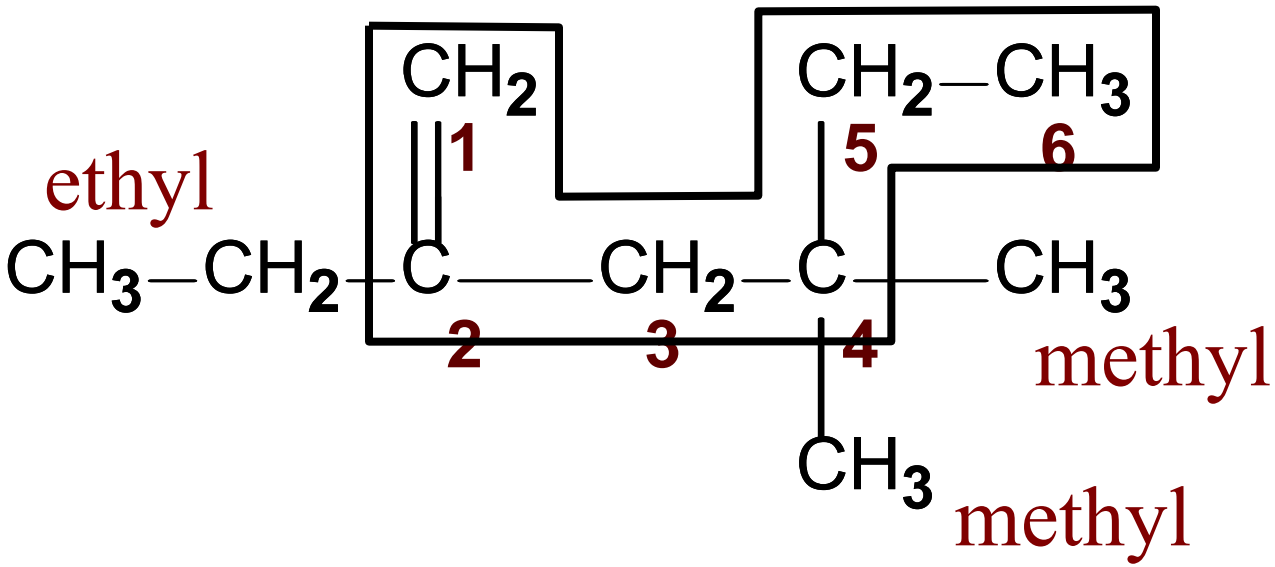
Naming Side Chains



Rule 7,8: group similar branches

2-ethyl-4-methyl-4-methyl-1-hexene

Naming Side Chains



Rule 7,8: group similar branches

2-ethyl-4,4-dimethyl-1-hexene

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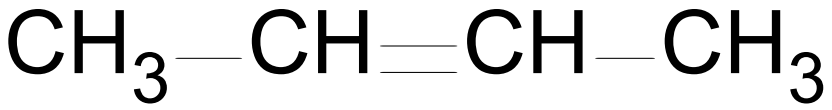
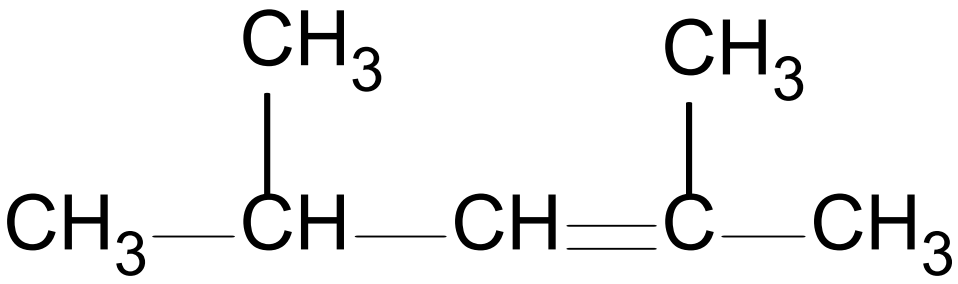
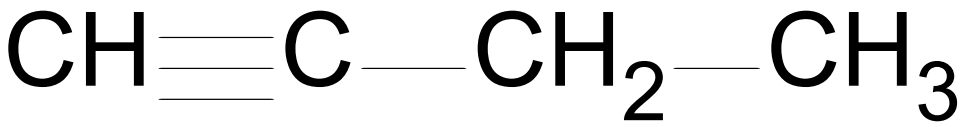
propene



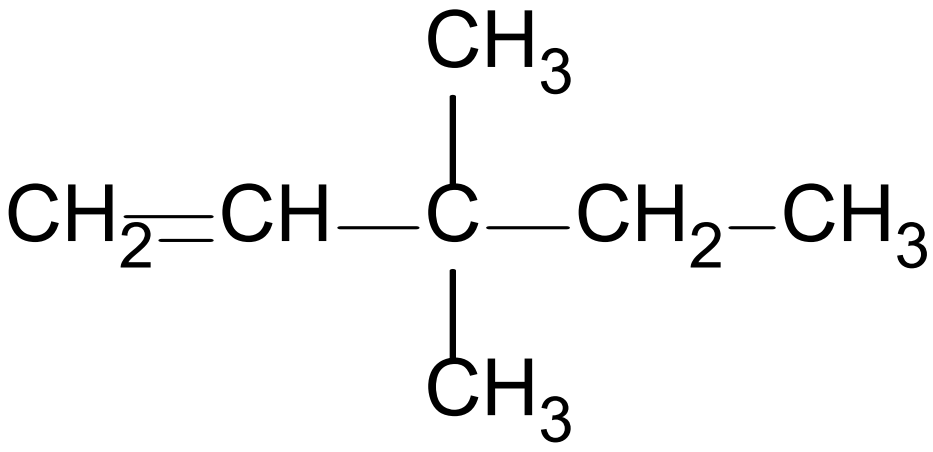
2-butene



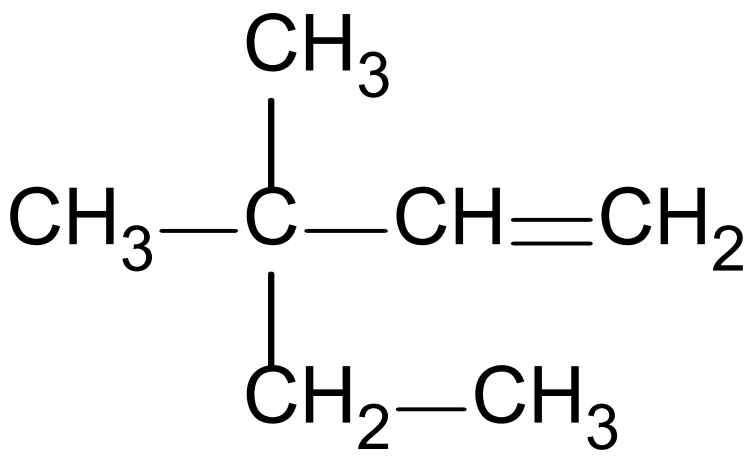
2,4-dimethyl-2-pentene



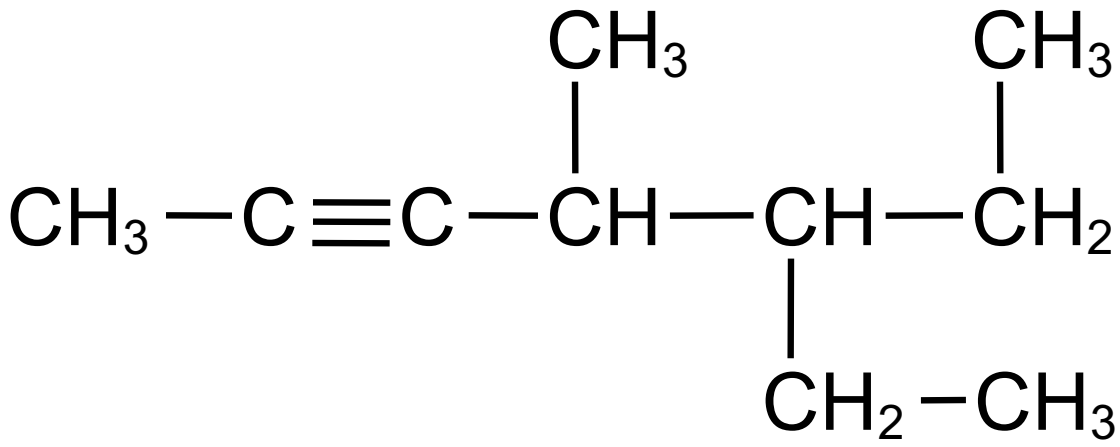
1-butyne



a) 3,3-dimethyl-1-pentene



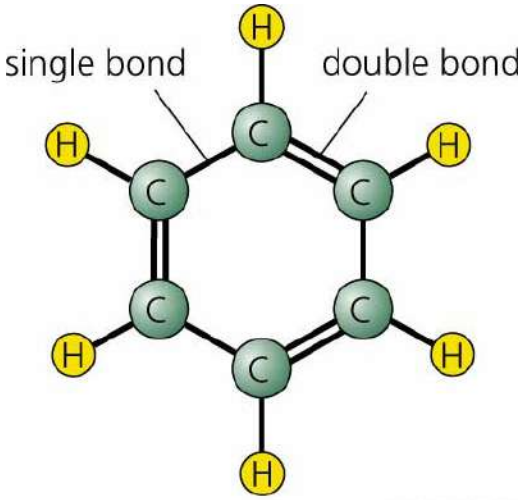
b) same

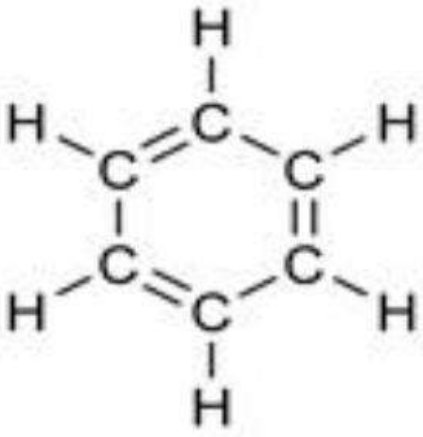


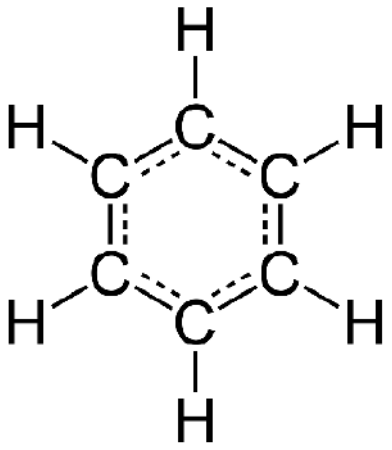
c) 5-ethyl-4-methyl-2-heptyne

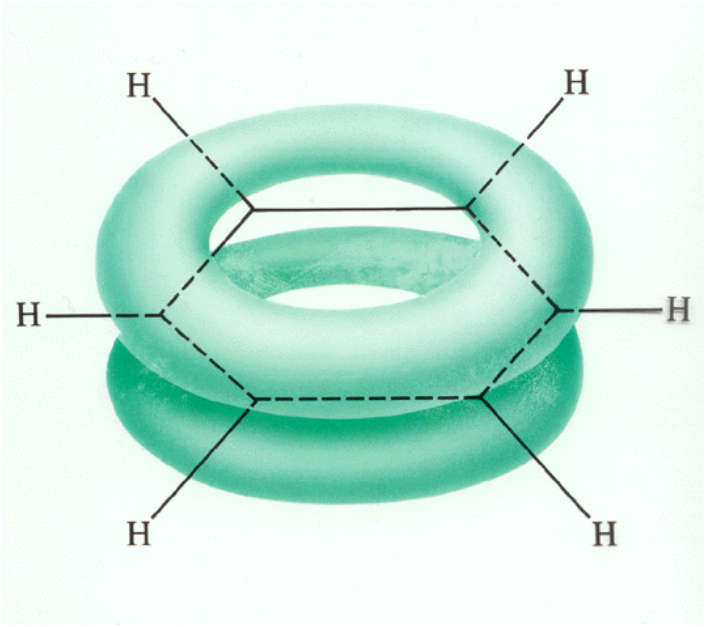
Aromatic Hydrocarbons

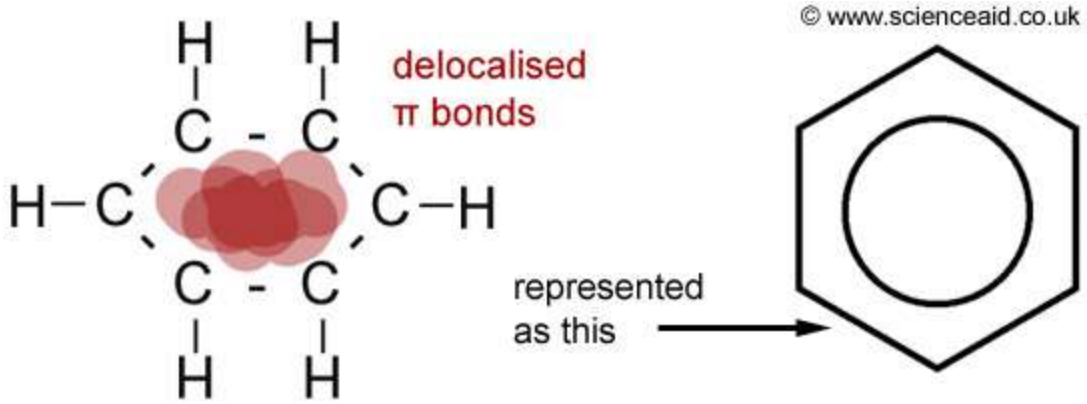
- Hydrocarbons with 6-membered carbon rings and delocalized electrons
- Benzene is the primary aromatic hydrocarbon







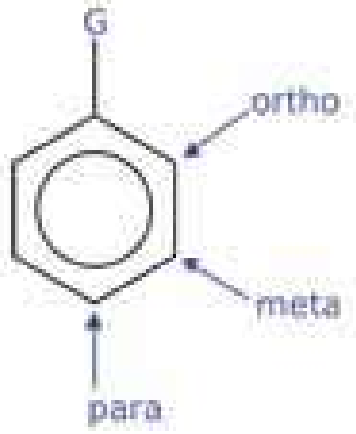

H
H
H
H
H
H


H
H
C - C
H–C
C–H
C - C
H
H
delocalised
π bonds
represented
as this
© www.scienceaid.co.uk

- Naming is similar
- Ex. Propyl benzene

- Ex. 1,3-dimethylbenzene

- Para, ortho, and meta are sometimes used to replace 1,2 (ortho)……1,3 (meta) …….and 1,4 (para)



Properties of aromatic compounds

- Chemically stable, less reactive than alkenes and alkynes
- Non-polar, therefore have limited solubility in water
- Used to be used as a nonpolar solvent until it was determined to be a carcinogen