Aliphatic and Aromatic Hydrocarbon Chemistry

Alkanes

- **Alkanes are compounds that are made up of only carbon and hydrogen atoms (i.e. *hydrocarbons*)**
- **All the carbon atoms in these compounds are sp^3 hybridized and consequently only sigma (single) bonds are found in these compounds and have a tetrahedral shape with a bond angle of 109° 28‘**
- **They are saturated hydrocarbons and form homologue series of the formula: C_nH_{2n+2}**

Naming of Alkanes

- **With the exception of the first four members of the series, the straight-chain (unbranched) alkanes are named by taking the Greek prefixes appropriate to the number of carbon atoms and adding the ending *'ane'*.**

Methane – CH_4	Hexane - CH_3-$(CH_2)_4$-CH_3
Ethane – CH_3-CH_3	Heptane - CH_3-$(CH_2)_5$-CH_3
Propane – CH_3-CH_2-CH_3	Octane - CH_3-$(CH_2)_6$-CH_3
Butane – CH_3-CH_2-CH_2-CH_3	Nonane - CH_3-$(CH_2)_7$-CH_3
Pentane – CH_3-$(CH_2)_3$-CH_3	Decane - CH_3-$(CH_2)_8$-CH_3

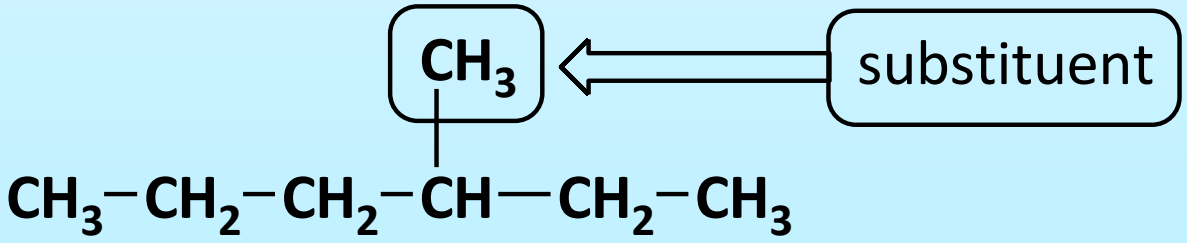
Naming of Alkanes

- **In these alkanes and if one of the terminal hydrogens is removed, the residual is an *alkyl group* and their name ends with *–yl***

CH_3-H ***Methane***	**becomes**	CH_3- ***methyl***
CH_3-CH_2-H ***Ethane***	**becomes**	CH_3-CH_2- ***ethyl***
CH_3-CH_2-CH_2-H ***Propane***	**becomes**	CH_3-CH_2- ***propyl***

Naming of Branch chain alkanes

- Branched alkanes have substituent groups other than hydrogen atom on the straight chain



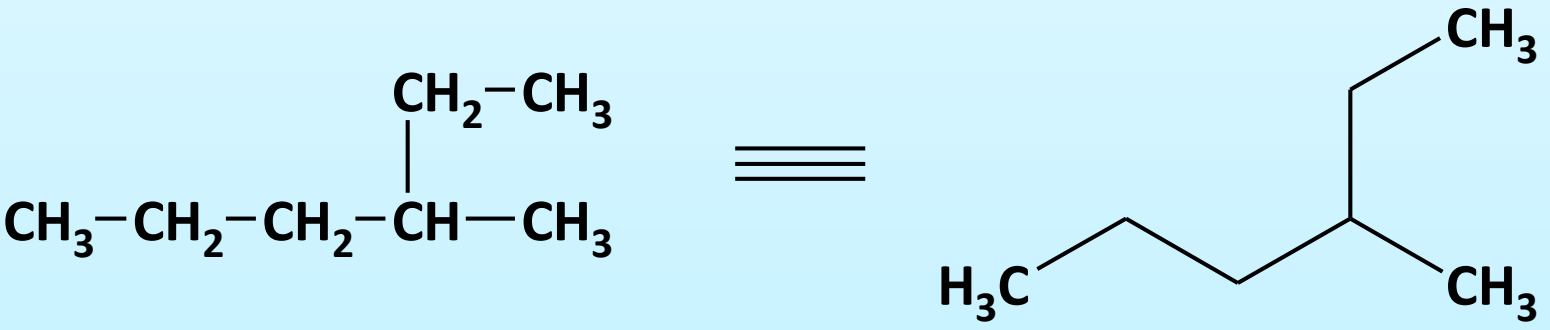
- Naming of these compounds follows certain rules
- Let us take a closer look at how these compounds are named including the one above?

Naming of Branch chain alkanes

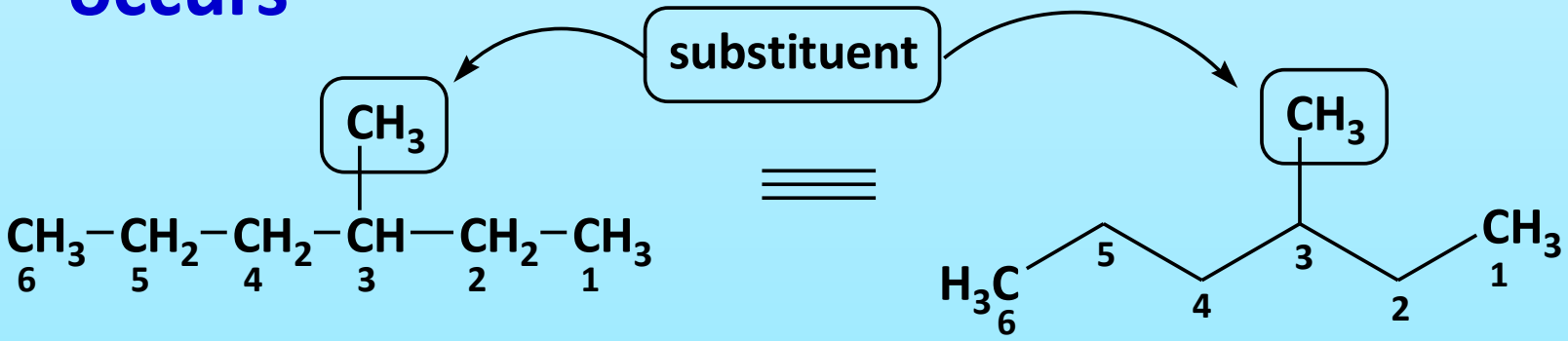
- **For alkanes that are branched, i.e. having a group other than a hydrogen atom on one of the non-terminal carbon atoms, they are named according to the following rules:**

1. **Locate the longest continuous chain of carbon atoms – this will form the name of the parent alkane *(warning – the longest chain may not always be obvious from how the formula is written)***

Naming of Branch chain alkanes

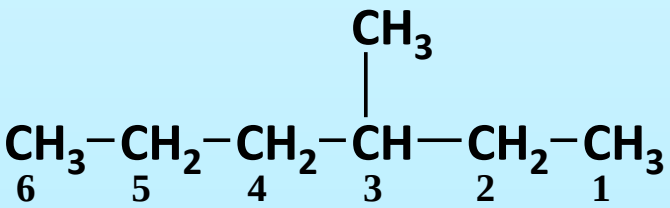


2. **Number the longest chain beginning with the end closest to the substituent, i.e. look for the shortest route to where branching occurs**



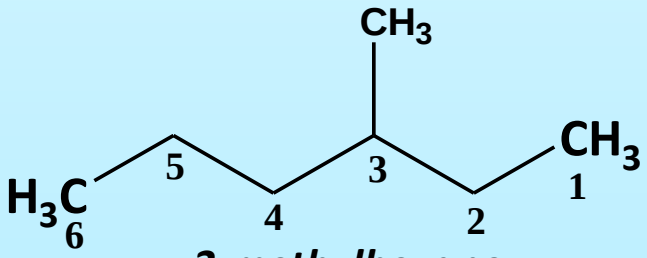
Naming of Branch chain alkanes

3. **Use the numbers obtained in Rule 2 to designate the location of the substituent on the chain**



3-methylhexane

≡

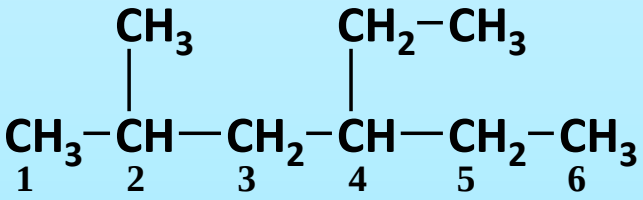


3-methylhexane

4. **When two or more substituents are present, give each substituent a number corresponding to its location on the longest chain using the same rules as shown above**

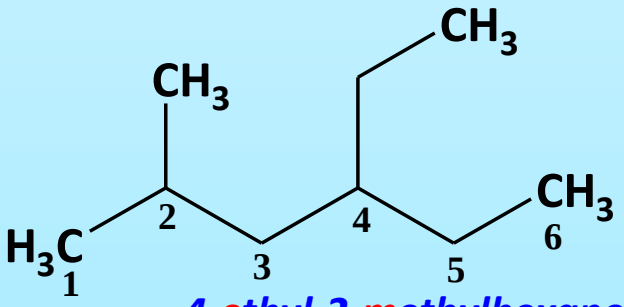
Naming of Branch chain alkanes

The substituents should be listed *alphabetically* (i.e. *ethyl* comes before *methyl*) and disregard the numbers. Also in deciding on alphabetical order, disregard multiplying prefixes such as "di" and "tri"



4-ethyl-2-methylhexane

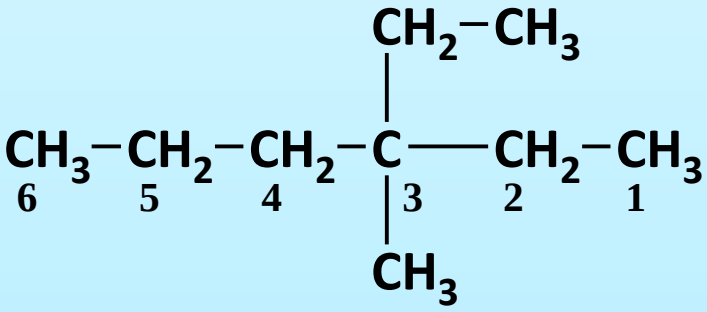
≡



4-ethyl-2-methylhexane

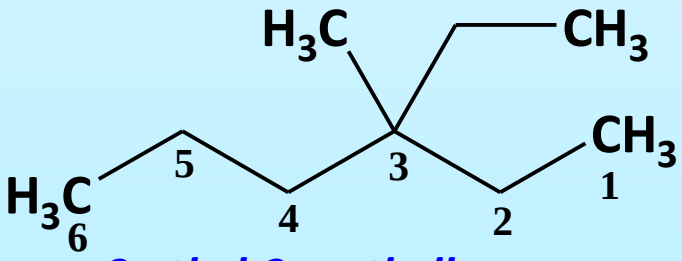
Naming of Branch chain alkanes

5. **When two substituents are on the same carbon, use the number twice**



3-ethyl-3-methylhexane

≡

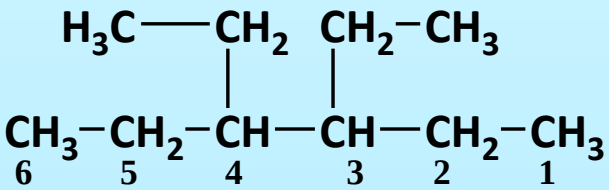


3-ethyl-3-methylhexane

6. **When two or more substituents are identical indicate this by the use of the prefixes *di-, tri-, tetra-* and so on.**

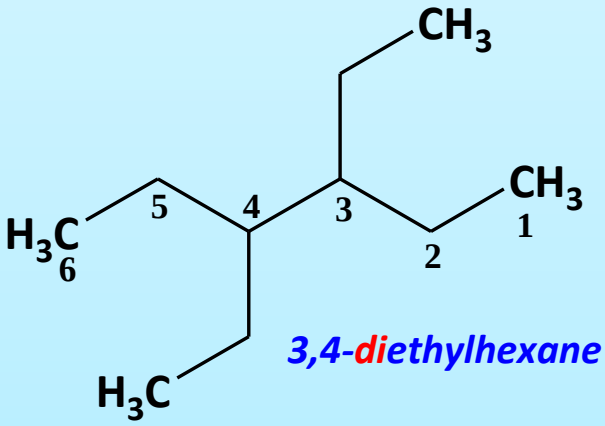
Naming of Branch chain alkanes

Make sure that every substituent has a number, using commas to separate them from each other



3,4-diethylhexane

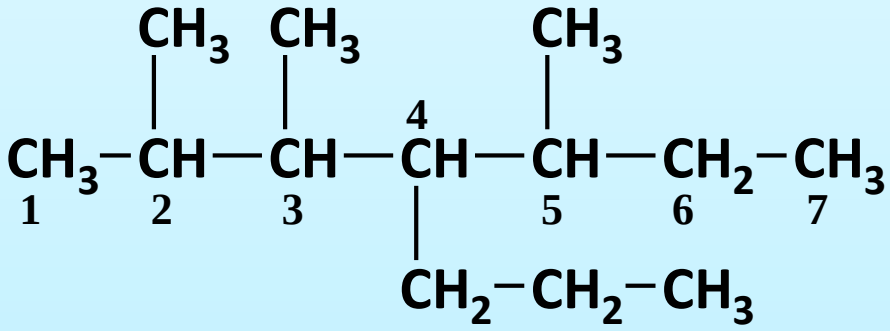
≡



3,4-diethylhexane

7. **When two chains of equal lengths compete for selection as the parent compound, choose the chain with the greater number of substituents**

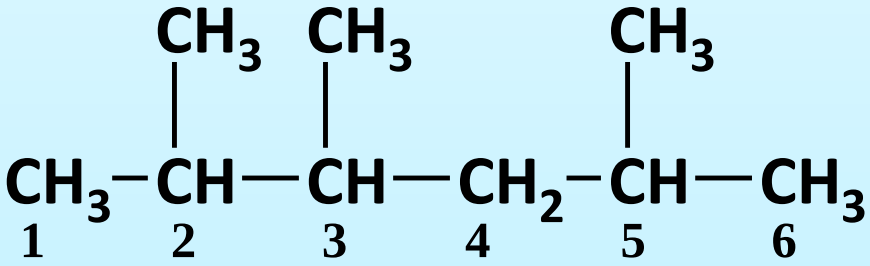
Naming of Branch chain alkanes



2,3,5-trimethyl-4-propylheptane

8. **When branching first occurs at an equal distance from either end of the longest chain, choose the name that gives the lower number at the first point of difference**

Naming of Branch chain alkanes



2,3,5-trimethylhexane

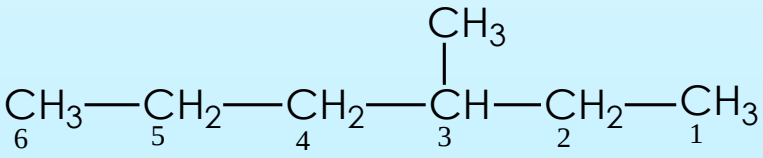
Earlier on we had a look at names of alkyl groups, which are derived from straight chain alkanes, i.e.

methane ⟹ methyl; ethane ⟹ ethyl

propane ⟹ propyl; butane ⟹ butyl etc…

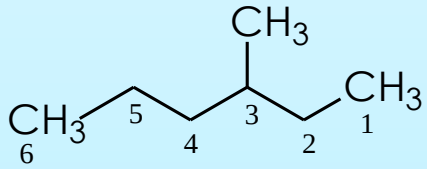
Naming of Branch chain alkanes

More examples:

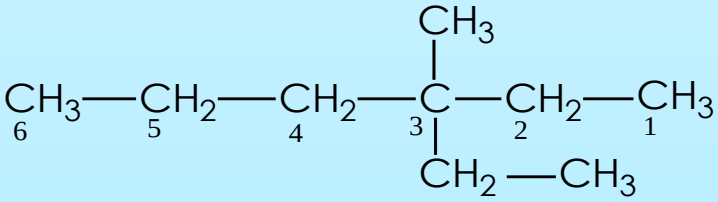


3-methylhexane

≡

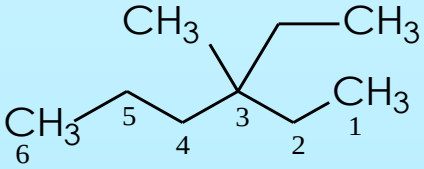


3-methylhexane

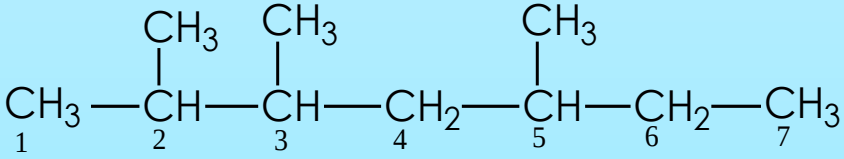


3-ethyl-3-methylhexane

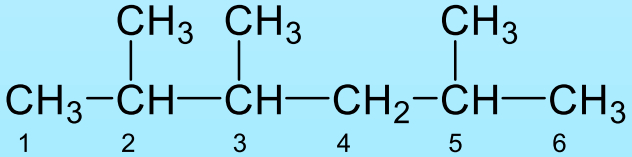
≡



3-ethyl-3-methylhexane



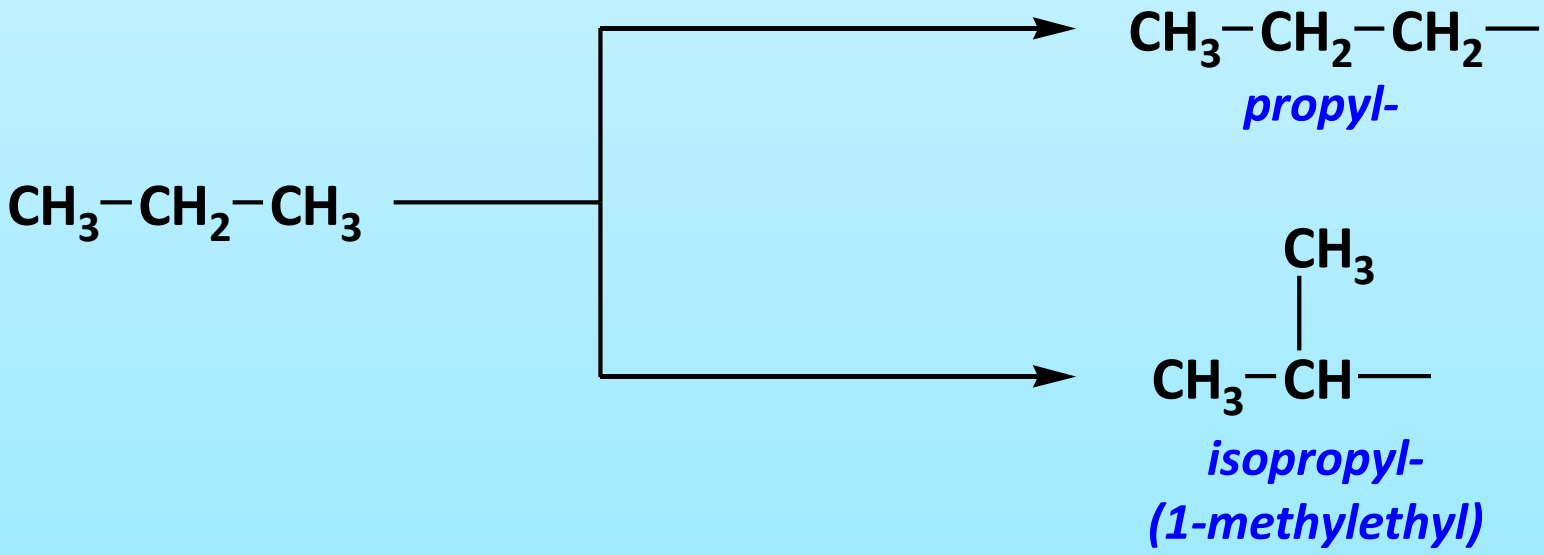
2,3,5-trimethylheptane



2,3,5-trimethylhexane
(not 2,4,5-trimethylhexane)

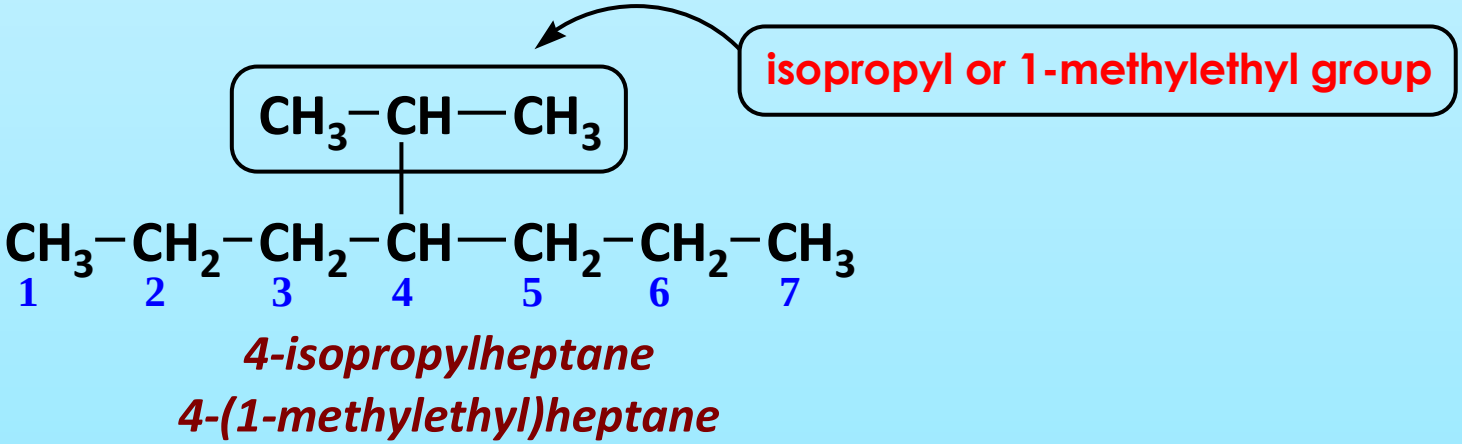
Naming of branched alkyl groups

- For alkanes with more than three carbon atoms, more than one derived group is possible
- Two alkyl groups can be derived from propane, e.g. the propyl group and the isopropyl group



Naming of branched alkyl groups

- Systematic naming of alkyl groups is very similar to that of branched-like alkanes with the provision that numbering always begins at the point where the groups are attached to the main chain
- The systematic name of the isopropyl is 1-methylethyl

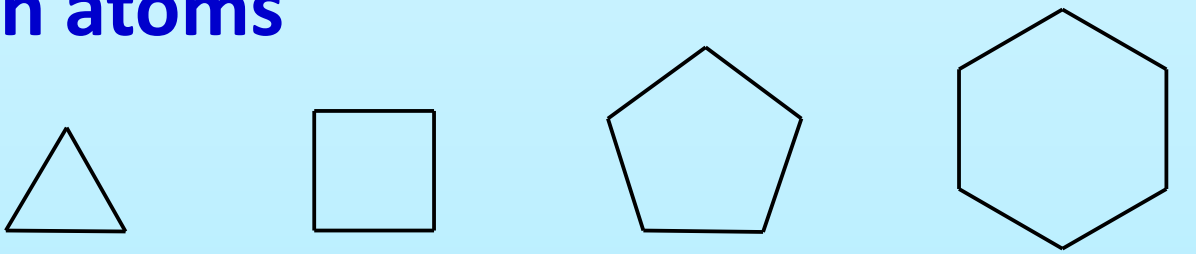


4-isopropylheptane

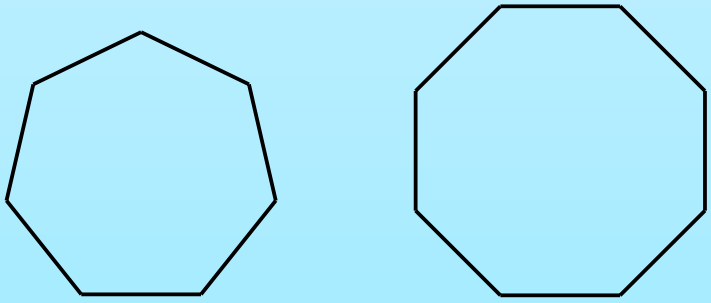
4-(1-methylethyl)heptane

Cycloalkanes

- **Cycloalkanes with only one ring are named by attaching a prefix *cyclo-* to the names of the alkanes possessing the same number of carbon atoms**



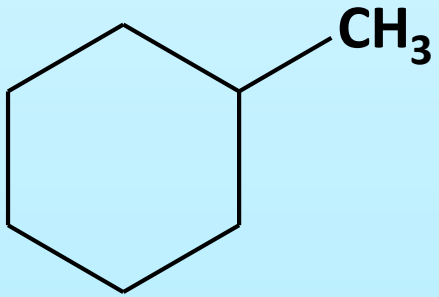
Cyclopropane ***Cyclobutane*** ***Cyclopentane*** ***Cyclohexane***



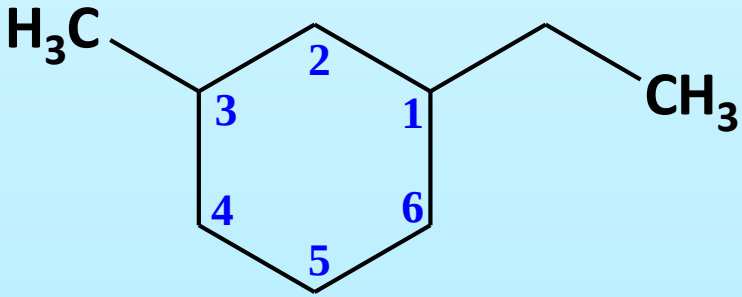
Cycloheptane ***Cyclooctane***

Cycloalkanes

- If a substituent is on the ring, the substituent's name is placed before the cycloalkane name



Methylcyclohexane



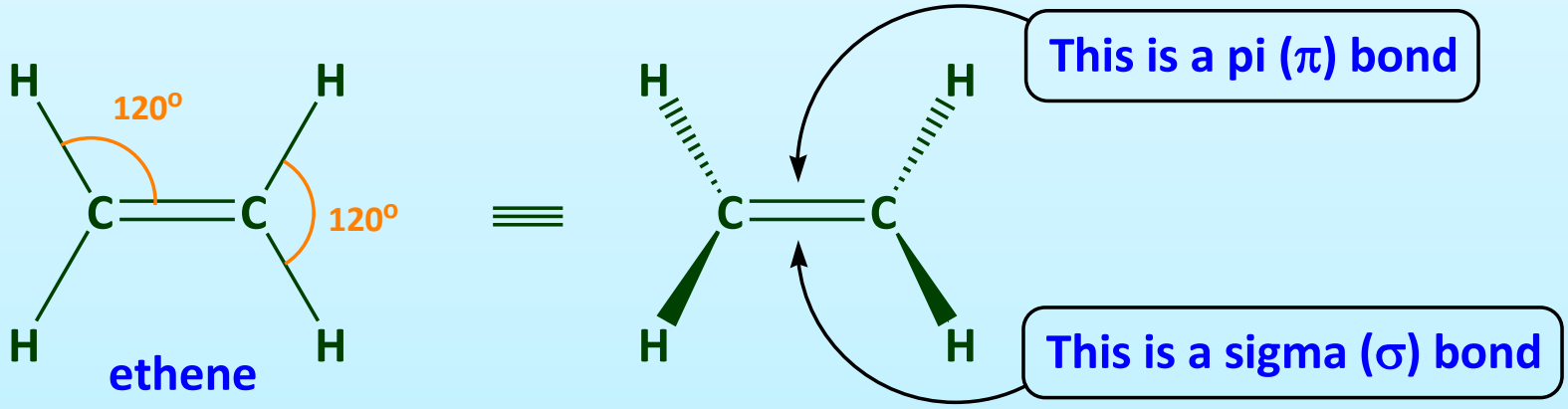
1-Ethyl-3-methylcyclohexane

- Notice that in the mono-substituted example no number is given but the di-substituted example has got numbers

Alkenes

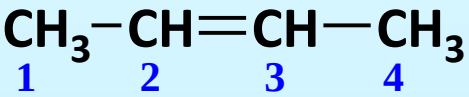
- Similar to alkanes, they form homologous series of unsaturated hydrocarbon compounds
- They contain a carbon-carbon double bond which follows the formula, C_nH_{2n}
- The carbon atoms involved in the double bond are sp^2 hybridized
- The double bonds consist of 1 σ bond and 1 π bond - its shape is trigonal planar with an angle of 120^o

IUPAC Naming of Alkenes

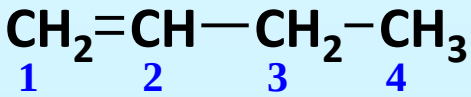


- An alkene is named by dropping the ending '-ane' from the corresponding alkane and replacing it with the suffix '-ene'.
- The position of the double bond(s) is specified by placing the appropriate number in the chain

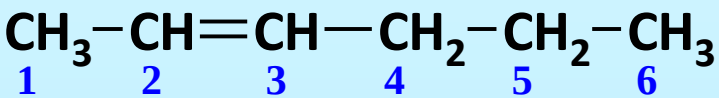
IUPAC Naming of Alkenes



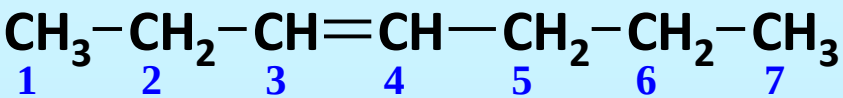
2-butene (or but-2-ene)



1-butene (or but-1-ene)

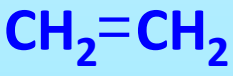


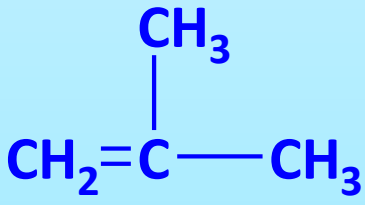
2-hexene (or hex-2-ene)



3-heptene (or hept-3-ene)

- **Many alkenes are still generally known by their common (trivial) names**





IUPAC:	**ethene**	**propene**	**2-methylpropene**
Common:	**ethylene**	**propylene**	**isobutylene**

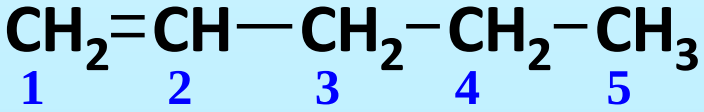
IUPAC Naming of Alkenes

- **The IUPAC rules for naming alkenes are very similar to those of naming alkanes**

1. **Determine the parent name by selecting the longest continuous chain that contains the double bond – once the longest chain has been identified, change the name by dropping the ‘-ane’ from the corresponding alkane’s name to ‘-ene’**

IUPAC Naming of Alkenes

For example – the parent name of a continuous chain with five carbons that contains the double bond is referred to as a pentene

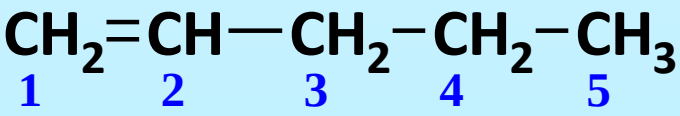


This is an example of a *pentene*

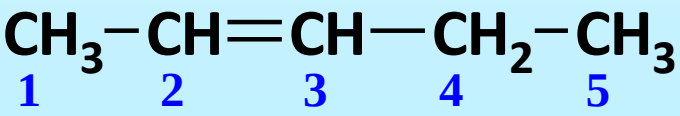
2. **Number the chain so as to include both carbon atoms of the double bond, and begin numbering at the end of the chain nearer to the double bond**

IUPAC Naming of Alkenes

Designate the location of the double bond by using the number of the first atom of the double bond as a prefix:



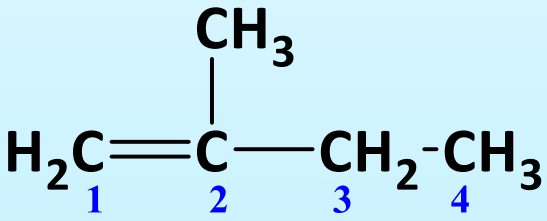
1-pentene
(not 4-pentene)



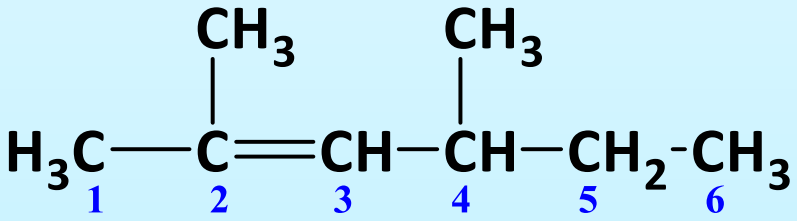
2-Pentene
(not 3-pentene)

3. **Indicate the location of the substituent groups by the number of the carbon atoms to which they are attached**

IUPAC Naming of Alkenes



2-methyl-1-butene
(not 3-methyl-3-butene)

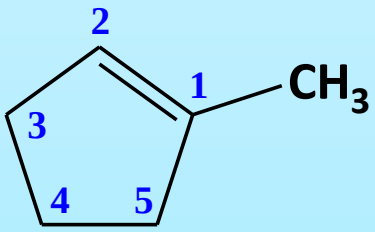


2,4-dimethyl-2-hexene
(not 3,5-dimethyl-4-hexene)

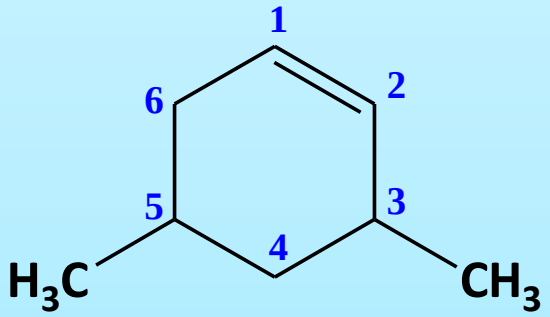
4. **Number substituted cycloalkenes in the way that gives the carbon atoms of the double bond the 1 and 2 positions and that gives the substituent group the lower numbers at the first point of difference**

IUPAC Naming of Alkenes

With substituted cycloalkenes, it is not necessary to specify the position of the double bond since it will always begin with C-1 and C-2



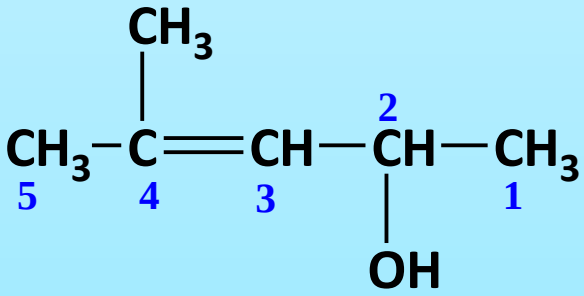
1-methylcyclopentene
(not 2-methylcyclopentene)



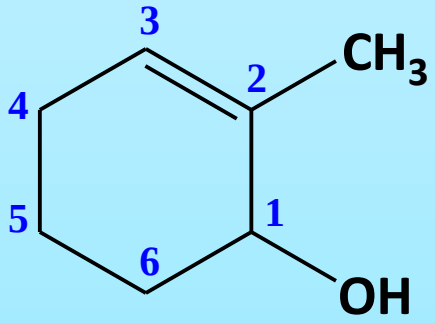
3,5-dimethylcyclohexene
(not 4,6-dimethylcyclohexene)

IUPAC Naming of Alkenes

5. **Compounds that contain a double bond and an alcohol group are named alkenols (cycloalkenols) and the carbon on the parent chain or cycloalkene to which the alcohol group is attached is given the lower number – in cycloalkenes, the position of the double has to be indicated**



4-methyl-3-penten-2-ol



2-methyl-2-cyclohexen-1-ol

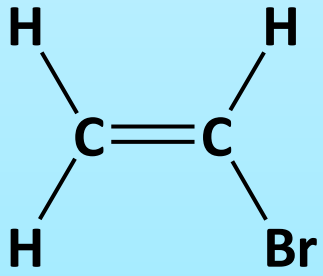
IUPAC Naming of Alkenes

6. **Two frequently encountered alkenyl groups are the *vinyl group and the allyl group***

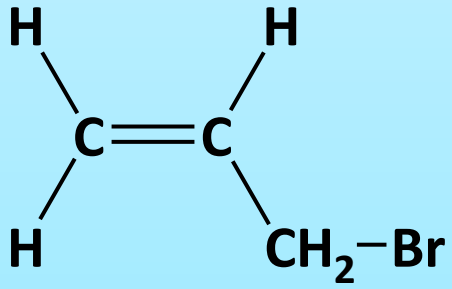
$CH_2{=}CH{-}$ — *The vinyl group*

$CH_2{=}CH{-}CH_2{-}$ — *The allyl group*

These names are used when old or common names are employed to name compounds – the following are examples:



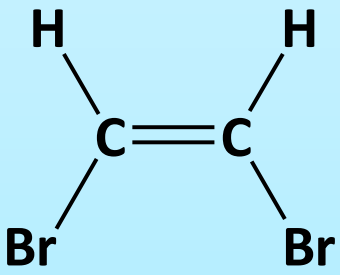
Bromoethene or vinylbromide



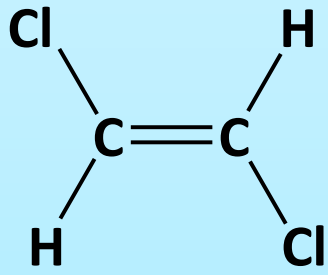
3-Bromopropene or allyl bromide

IUPAC Naming of Alkenes

7. **If two identical groups are on the same side of the double bond, the compound can be designated as *cis*; if they are on opposite sides, it can be designated as *trans***



***cis*-1,2-dibromoethene**

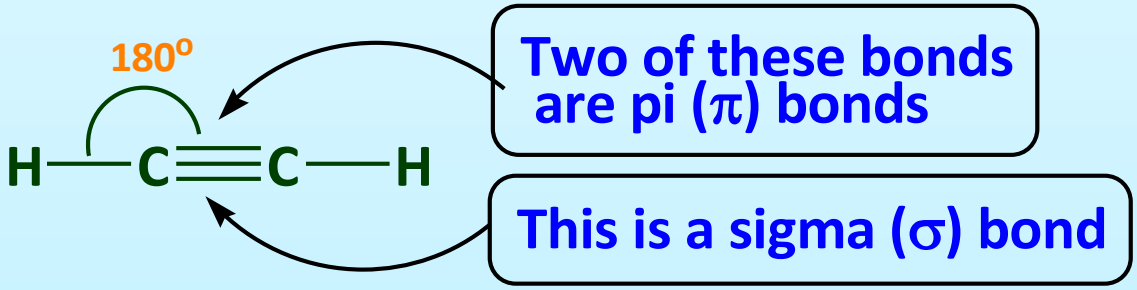


***trans*-1,2-dichloroethene**

Alkynes

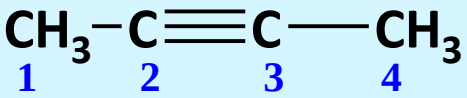
- Similar to alkanes and alkenes, they form homologous series of unsaturated hydrocarbon compounds
- They contain a carbon–carbon triple bond which follows the formula, C_nH_{2n-2}
- The carbon atoms involved in the triple bond are sp^1 hybridized
- The triple bonds consist of 1 σ bond and 2 π bonds - it's geometrical shape is linear with an angle of 180^o

IUPAC Naming of Alkynes

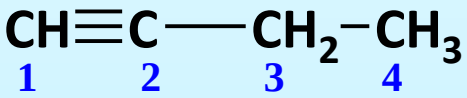


- An alkyne is named by dropping the ending '-ane' from the corresponding alkane and replacing it with the suffix '-yne'.
- Again the position of the triple bond(s) is specified by placing the appropriate number of the first alkyne carbon in the chain

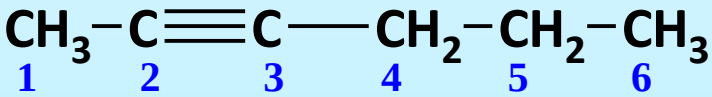
IUPAC Naming of Alkynes



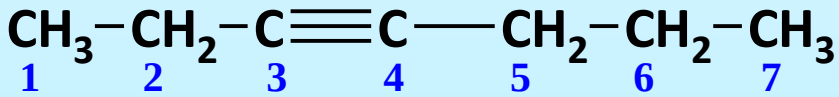
2-butyne (or but-2-yne)



1-butyne (or but-1-yne)



2-hexyne (or hex-2-yne)



3-heptyne (or hept-3-yne)

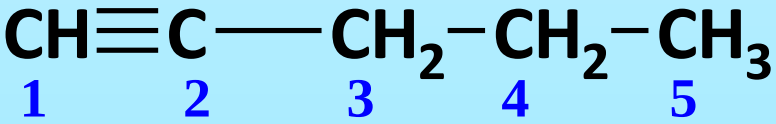
- **The IUPAC rules for naming alkynes are very similar to those for naming alkanes and alkenes**

1. **As with alkenes determine the parent name by selecting the longest continuous chain that contains the triple bond**

IUPAC Naming of Alkynes

Once the longest chain has been identified, change the name by dropping the '-ane' from the corresponding alkane's name to '-yne'

For example – the parent name of a continuous chain with five carbons that contains the triple bond is referred to as a pentyne

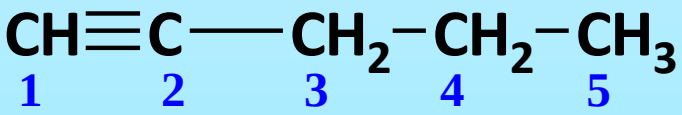


This is an example of a *pentyne*

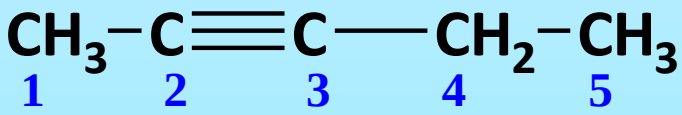
IUPAC Naming of Alkynes

2. **Number the chain so as to include both carbon atoms of the triple bond, and begin numbering at the end of the chain nearer to the triple bond**

Designate the location of the triple bond by using the number of the first atom of the triple bond as a prefix:



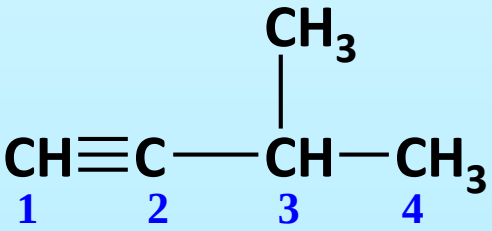
1-pentyne
(not 4-pentyne)



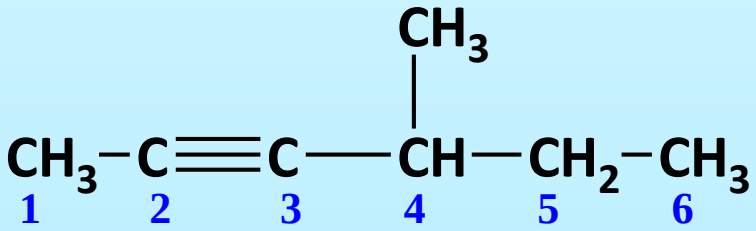
2-Pentyne
(not 3-pentyne)

IUPAC Naming of Alkynes

3. **Indicate the location of the substituent groups by the number of the carbon atoms to which they are attached**



3-methyl-1-butyne
(not 2-methyl-3-butyne)



4-methyl-2-hexyne
(not 3-methyl-4-hexyne)

4. **As we saw with alkenes, when a heteroatom is present on the molecule, the heteroatom takes priority in the naming the molecule**