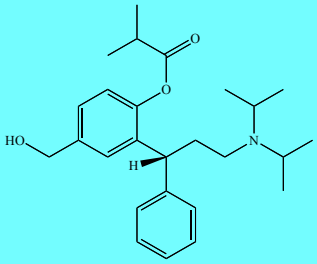
Molecular Representations, Nomenclature, and Isomers





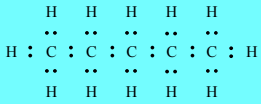
Isobutyric acid 2-((*R*)-3-diisopropylamine-1 -phenylpropyl)-4-(hydroxymethyl) phenyl ester

Fesoterodine

Molecular Representations

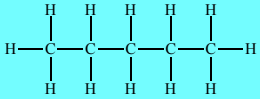
Several ways to represent structure of organic molecules....

Lewis dot structure



Cumbersome

Kekulé structure



Still cumbersome

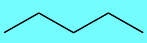
Condensed structure

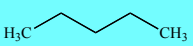
$CH_3CH_2CH_2CH_2CH_3$

Often unclear

Bond-line structure

- Carbon framework = zigzag lines
- End of each line = carbon
- H omitted (unless carbon shown as C)





Nomenclature

Different people = different names

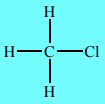

Hey you


Hey you


Hey you

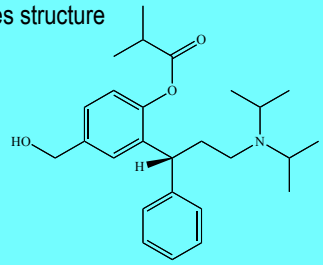
Different molecules need different names

- **Nomenclature**: Naming scheme that describes structure
- Names can be simple or complex
- Most molecules have several names



Chloromethane

Methyl chloride



Isobutyric acid 2-((*R*)-3-diisopropylamine-1 -phenylpropyl)-4-(hydroxymethyl) phenyl ester

Fesoterodine

Nomenclature Rules

Let's start with alkanes...

What is the rule for these names?

$CH_3CH_2CH_2CH_2CH_3$	Pentane	C_5H_{12}
$CH_3CH_2CH_2CH_2CH_2CH_3$	Hexane	C_6H_{14}
$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	Octane	C_8H_{18}

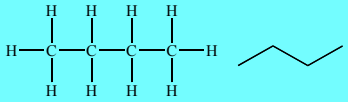
Answer: **Number of carbons + *ane***

Structure	Formula	Name	Structure	Formula	Name
CH_4	CH_4	Methane	$CH_3(CH_2)_5CH_3$	C_7H_{16}	Heptane
CH_3CH_3	C_2H_6	Ethane	$CH_3(CH_2)_6CH_3$	C_8H_{18}	Octane
$CH_3CH_2CH_3$	C_3H_8	Propane	$CH_3(CH_2)_7CH_3$	C_9H_{20}	Nonane
$CH_3CH_2CH_2CH_3$	C_4H_{10}	Butane	$CH_3(CH_2)_8CH_3$	$C_{10}H_{22}$	Decane
$CH_3CH_2CH_2CH_2CH_3$	C_5H_{12}	Pentane	$CH_3(CH_2)_9CH_3$	$C_{11}H_{24}$	Undecane
$CH_3CH_2CH_2CH_2CH_2CH_3$	C_6H_{14}	Hexane	$CH_3(CH_2)_{10}CH_3$	$C_{12}H_{26}$	Dodecane

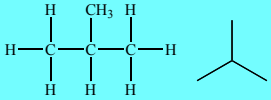
Isomers

More than one way to connect the atoms of a certain formula?

- CH_4, C_2H_6, C_3H_8: Only one sequence to arrange the atoms *Verify with models*
- C_4H_{10}: Two possible atom sequences



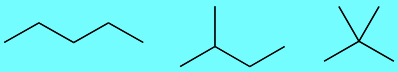
C_4H_{10} Butane



C_4H_{10} Name = ?

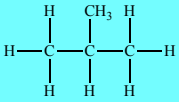
Isomers: Molecules with same chemical formula but different structure

Constitutional isomers: Isomers that differ in sequence of atom connectivity

Example: Pentane isomers 

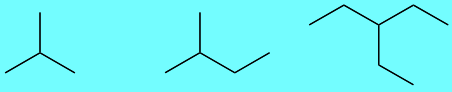
Substituents

Substituent: An atom or group other than hydrogen on a molecule.

 Name?

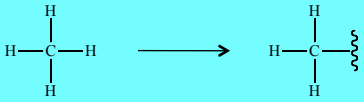
How to name alkanes with substituents?

What is the rule for these names?

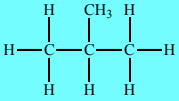


Methylpropane Methylbutane Ethylpentane

Answer: **Substituent name = parent alkane – *ane* + *yl***

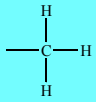
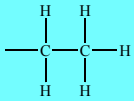
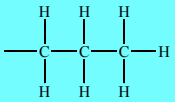
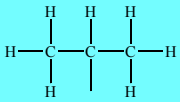


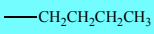
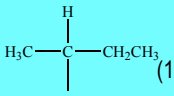
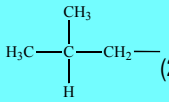
Methane Methyl group



Substituent Names

Substituent name = parent alkane – *ane* + *yl*

Parent alkane	Substituent structure	Substituent name
Methane		Methyl
Ethane		Ethyl
Propane		Propyl
Propane		Isopropyl

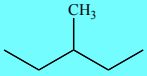
Parent alkane	Substituent structure	Substituent name
Butane		Butyl
Butane		*Sec*-butyl (1-methylpropyl)
Butane		Isobutyl (2-methylpropyl)
Butane		*Tert*-butyl (2-methyl-2-propyl)

Locants

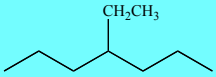
What happens when substituents can be at different positions on the parent chain?

What is the rule for these names?

2-Methylpropane



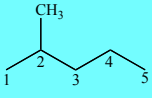
3-Methylpentane



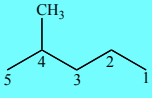
4-Ethylheptane

Answer:

•Number chain so substituent is on lowest number carbon



2-Methylpentane



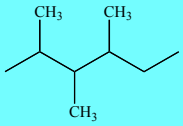
4-Methylpentane

Multiple Substituents

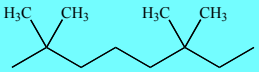
What happens when the parent chain has multiple substituents?

What is the rule for these names?

2,2-Dimethylpropane



2,3,4-Trimethylhexane

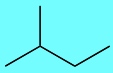


2,2,6,6-Tetramethyloctane

Answer:

- Di = two of same substituent
- Tri = three of same substituent
- Tetra = four of same substituent

When one substituent, mono not included:

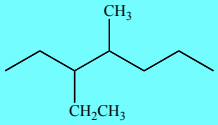


2-Methylbutane

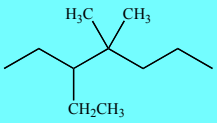
2-Monomethylbutane

Multiple Substituents: Alphabetizing

Multiple substituents may lead to multiple names:



3-Ethyl-4-methylheptane *Correct*
4-Methyl-3-ethylheptane *Incorrect*

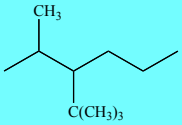


4,4-Dimethyl-3-ethylheptane *Incorrect*
3-Ethyl-4,4-dimethylheptane *Correct*

What rule is operating in this case?

Answer:

- Ethyl beats methyl
- Ethyl beats dimethyl
- Ignore *sec* and *tert*

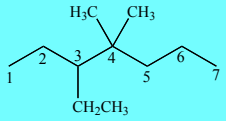


3-*Tert*-butyl-2-methylhexane

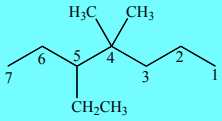
2-Methyl-3-*tert*-butylhexane

Multiple Substituents: Locant Numbering

When there are multiple substituents, number chain to give lowest locant total:



4,4-Dimethyl-3-ethylheptane



4,4-Dimethyl-5-ethylheptane

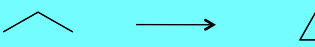
Cycloalkanes

Alkanes can also form rings; called **cycloalkanes**. Examples:

Cyclopropane Cyclopentane Cyclohexane

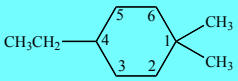
What naming rule is operating for these cycloalkanes?

Answer:



Propane - acyclic
Three carbons

Cyclopropane – cyclic
Three carbons

Naming rules otherwise same as acyclic alkanes. Example: 

1,1-Dimethyl-4-ethylcyclohexane

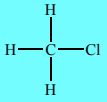
Other Substituents

Nomenclature applies to more than just alkanes and cycloalkanes.

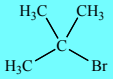
Many other substituent rules exist. Example:

Halogens: F = fluoro; Cl = chloro; Br = bromo, and I = iodo

- In simple cases, write halide name followed by substituent name



Chloromethane
Methyl chloride



2-Bromo-2-methylpropane
Tert-butyl bromide

Many other rules
Many other substituents → More details
More examples → Klein and Brown & Foote