ORGANIC CHEMISTRY 1 LECTURE GUIDE 2019

BY RHETT C. SMITH

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Organic Chemistry 1
Lecture Guide 2019

By Rhett C. Smith, Ph.D.

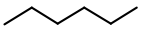
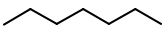
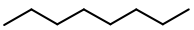
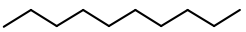
Companion Books from the Proton Guru:

Organic Chemistry 1 Reactions and Practice Problems 2019

by Rhett C. Smith

Organic Chemistry 1 Primer 2019,

by Rhett C. Smith, Andrew G. Tennyson, and Tania Houjeiry

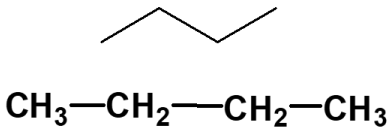
CH_4	
CH_3CH_3	
$CH_3CH_2CH_3$	
$CH_3(CH_2)_2CH_3$	
$CH_3(CH_2)_3CH_3$	
$CH_3(CH_2)_4CH_3$	
n-C_7H_{16}	
n-C_8H_{18}	
n-C_9H_{20}	
n-$C_{10}H_{22}$	

Notes

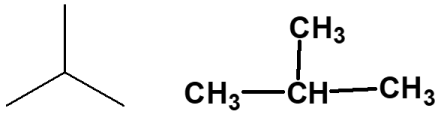
Constitutional Isomers-

C_4H_{10}

linear alkanes
('*n*ormal' alkanes)



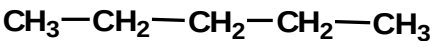
branched alkanes

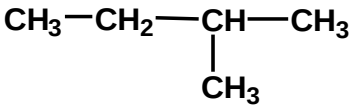


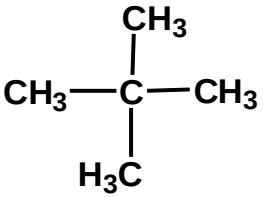
Lighter fluid is 5% *n*-butane and 95% isobutane

Notes

C_5H_{12}

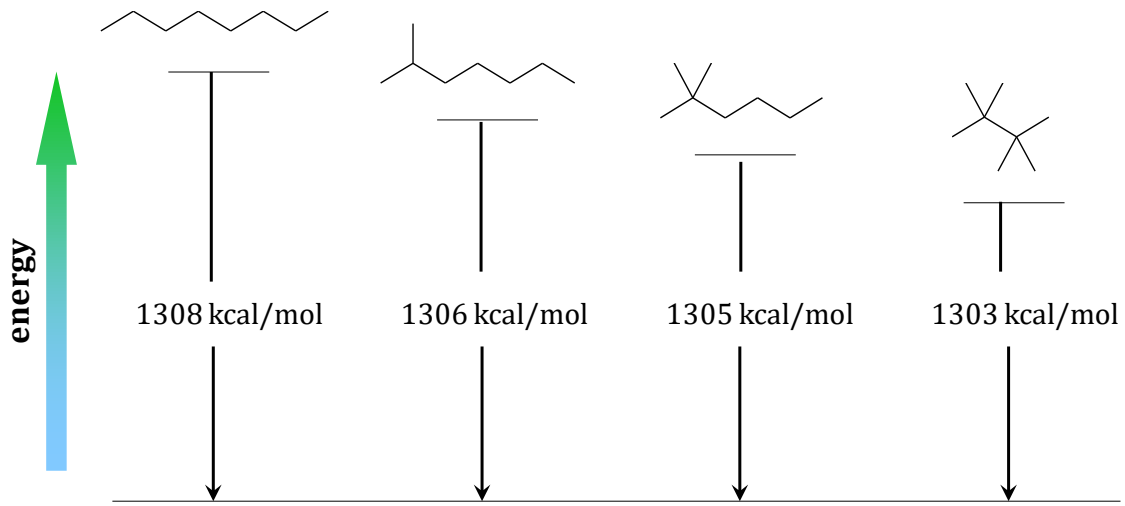






Notes

Heats of combustion (ΔH_c) for burning C_8H_{18} isomers:



The **more branching**, the **less heat released**, so

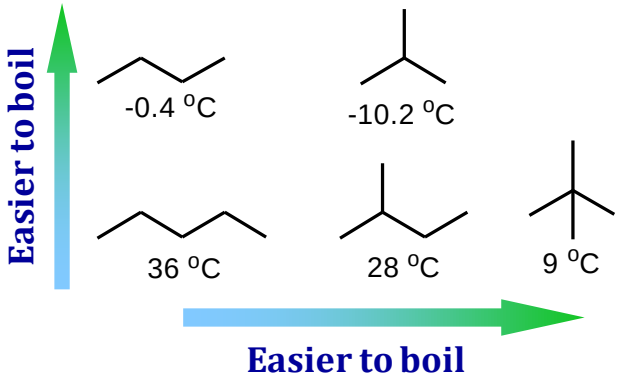
more branched =

Notes

Easier to boil

alkane	bp
CH_4	-160ºC
C_2H_6	-89
C_3H_8	-42
n-C_4H_{10}	-0.4
n-C_5H_{10}	36

Compare linear to branched alkanes:



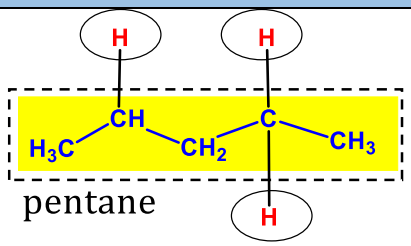
The **lighter** or **more branching**, the **less intermolecular force**, so

more branched =

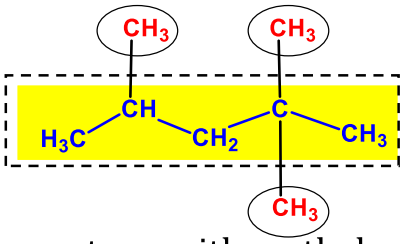
Lighter =

Notes

Substituents can Modify a Parent Alkane



pentane



pentane with methyl groups substituted for some of the hydrogens

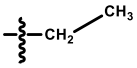
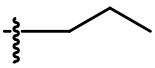
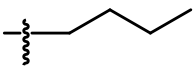
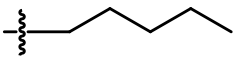
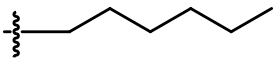
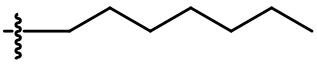
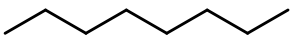
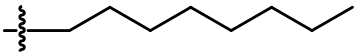
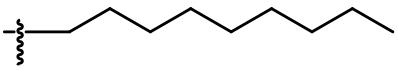
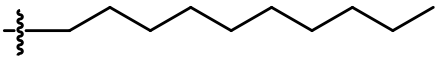
Substituent:

Substituents that occur frequently in molecules of interest are given names to simplify naming a complex molecule.

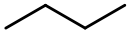
Of course there are substituents other than methyl groups we can put on to a molecule …

Notes

Lecture Topic I.14: Nomenclature of Alkanes, Alkyl halides, Alcohols and Cycloalkanes
Naming Linear Alkyl Substituents

meth**ane**			meth**yl**
eth**ane**			eth**yl**
prop**ane**			n-prop**yl**
n-but**ane**			n-but**yl**
n-pent**ane**			n-pent**yl**
n-hex**ane**			n-hex**yl**
n-hept**ane**			n-hept**yl**
n-oct**ane**			n-oct**yl**
n-non**ane**			n-non**yl**
n-dec**ane**			n-dec**yl**

Notes

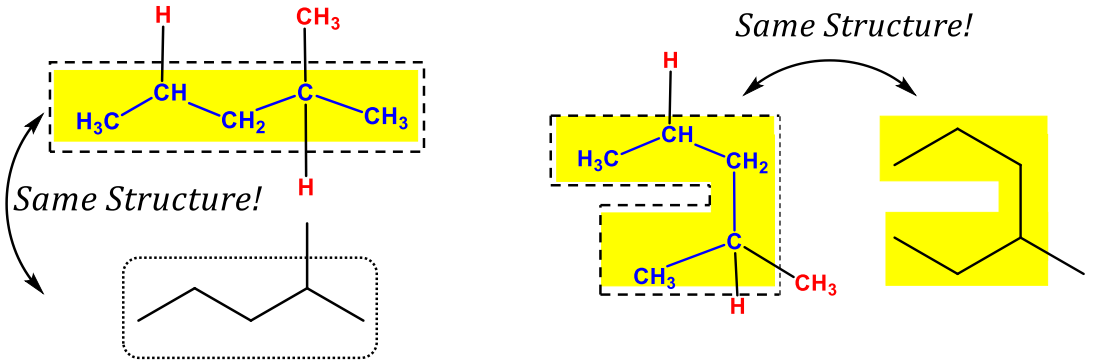
propane		*n*-propyl	"*n*-" indicates it is "normal", linear
propane		isopropyl	"*iso*-" indicates it has a 3-C, Y-shaped unit
n-butane		*n*-butyl	"*n*-" indicates it is "normal", linear
n-butane		*sec*-butyl	"*sec*-" indicates it is substituted at the secondary carbon
isobutane		isobutyl	"*iso*-" indicates it has a 3-C, Y-shaped unit
isobutane		*tert*-butyl	"*tert*-" indicates substitution at the tertiary carbon

Notes

Your step-by-step guide

1.

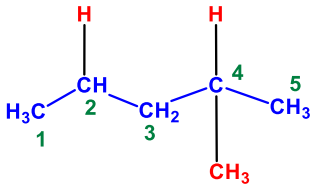
This is the 'parent chain'; the other stuff on the parent chain will be named as substituents. Be aware that there are many ways to draw the same molecule:



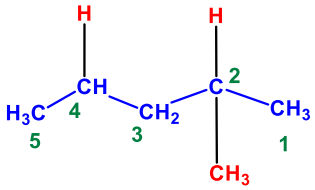
This is pentane, with one methyl ($-CH_3$) substituent … regardless of how it is drawn!

Notes

2. Number the carbon atoms in the 'parent chain' in the way that gives the lowest number to the substituent closest to an end of the parent chain.



or



?

A

B

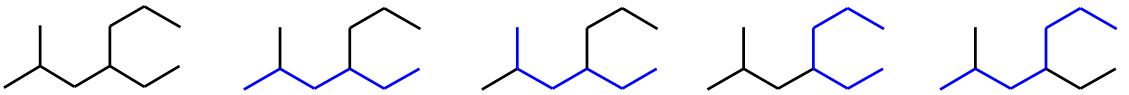
C

This molecule is properly named

Notes

1. Find the longest chain

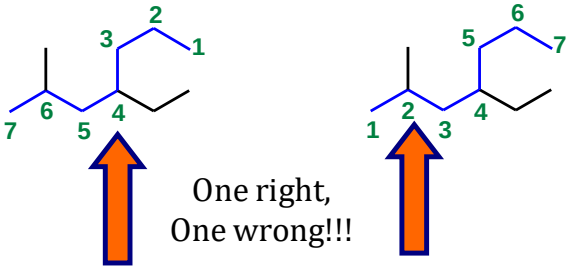
alkane **possible parent chains:**



#C's: **6** **6** **6** **7**

2. Number the parent chain to give lowest number to substituent closest to end

possible numbering schemes:

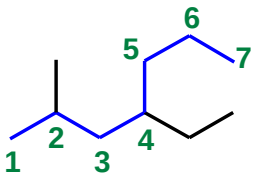


One right,
One wrong!!!

Ⓐ Ⓑ

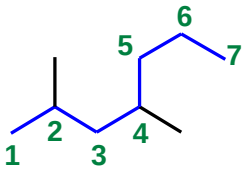
Notes

3. With more than one type of substituent,



We could name it
2-methyl-4-ethylheptane
or
4-ethyl-2-methylheptane

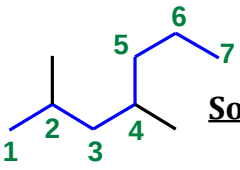
Since 'ethyl' is alphabetically before 'methyl', this molecule is properly named



Now consider this closely related molecule, in which the ethyl group is changed to a methyl group. The numbering and parent chain are the same, but now we have two methyl groups; we need to apply the next rule …

Notes

4. If more than one of the same substituent are present on your parent chain, use di, tri, tetra, etc. prefixes to denote this (**these prefixes do not count when alphabetizing.** Neither do the *n*-, *sec*-, or *tert*- prefixes.



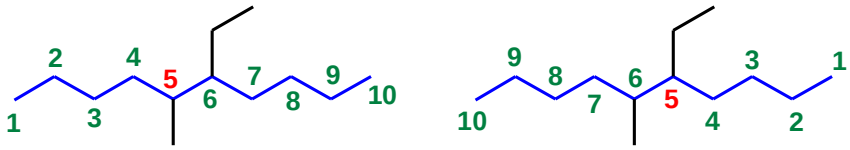
So, we call this

NOT
2-methyl-4-methylheptane
or
4-methyl-2-methylheptane

Incorrect names!

Notes

There are even more potential complications that could trip us up; consider:



We've easily found the parent chain (decane), and we try to find the right numbering scheme; but either way we count, the first substituent is at the **5** position; which is right?
We need the next rule:

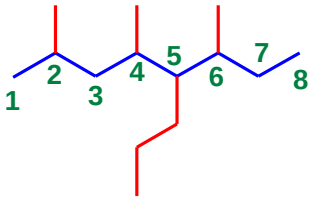
5. If numbering leads to the same "lowest number" substituent in both directions the correct numbering:

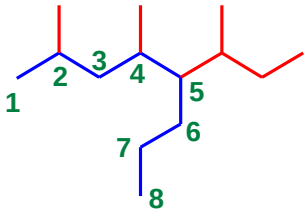
In this case, ethyl is alphabetically before methyl, so ethyl is given the 5:

This molecule is properly named:

Notes

The previous example showed you how to deal with substituent numbering issues; but what if you have trouble identifying the parent chain to begin with? Consider:





T**wo** possible octane parent chains; which is right? We need another rule.

6. If you find two different possible parent chains of the same length,

The one on the left has more substituents, so we use that parent chain.

This molecule is properly named:

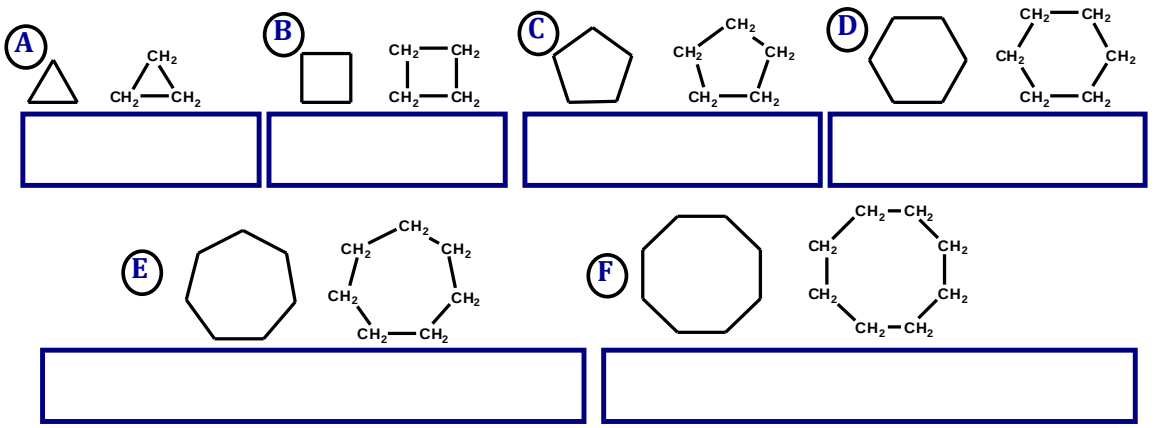
Notes

Your step-by-step guide to alkane nomenclature

1. Find the longest chain. This is the 'parent chain'; the other stuff on the parent chain will be named as substituents. Be aware that there are many ways to draw the same molecule.
2. Number the carbon atoms in the 'parent chain' in the way that gives the lowest number to the substituent closest to an end of the parent chain.
3. With more than one type of substituent, name in alphabetical order.
4. If more than one of the same substituent are present on your parent chain, use di, tri, tetra, etc. prefixes to denote this (these prefixes do not count when alphabetizing, though; neither do the n-, sec-, or tert- prefixes)
5. If numbering leads to the same lowest number substituent in both directions the correct numbering gives the lowest number to the substituent that is first alphabetically.
6. If you find two different possible parent chains of the same length, you choose the one with more substituents coming off of it.

Notes

Cyclic versions of alkanes are called cycloalkanes, and are named by the prefix used in the linear alkane with the same number of carbon atoms:

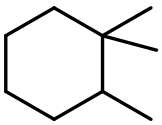


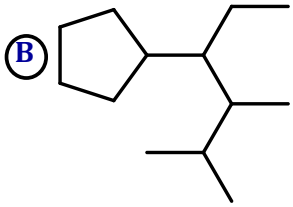
Of course, cycloalkanes can have substituents as well, and we need to know how to name substituted cycloalkanes.

Notes

Armed with our knowledge of naming branched alkanes, naming cycloalkanes is pretty straightforward. We can use the cycloalkane as the parent chain (if it is longest) and follow numbering/alphabetizing rules from there.

<u>An additional rule for naming cycloalkanes:</u>
If there is a possible parent chain on the cycloalkane that is longer than the # of carbons in the cycloalkane, use that as the parent chain, and name the cycloalkane as a substituent. For example:

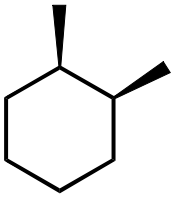
A 

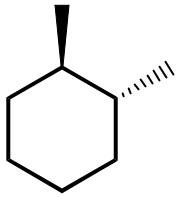
B 

Notes

Depending on where we put the methyl substituents, we have two different **configurational isomers**.

A configurational isomer in which substituents are on the same side (both 'up' in this case) is referred to as a ***cis-*** isomer, while a configurational isomer with substituents on opposite sides is referred to as the ***trans-*** isomer.

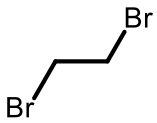




Notes

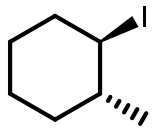
For alkyl halides, name the compound using the rules for naming alkanes and cycloalkanes, and treat the halides as substituents:

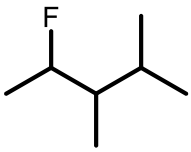
CCl_2H_2 dichloromethane



1,2-dibromoethane

-F = Fluoro
-Cl = Chloro-
-Br = Bromo-
-I = Iodo-





Notes

For alcohols, use the rules for naming alkanes and cycloalkanes as a starting point, with the following adjustments:

1. replace the “e” at the end of the alkane name with “ol”.

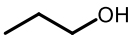
2. The alcohol is always given the lowest possible number. Note that this means that the alcohol is always given the “1” position in cycloalkanes (so, no need to add a number; we know it’s always 1).

3. Place the number indicating the position of the alcohol directly before the parent chain name (which now ends in “ol”).

Notes

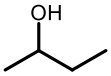
CH_3OH Methanol

CH_3CH_2OH Ethanol

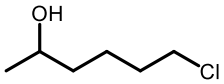


1-propanol
(or *n*-propanol)

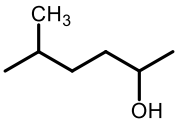
2-propanol
(or isopropanol)

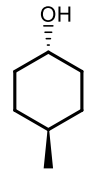
A 

2-methyl-2-propanol
(or *tert*-butanol)

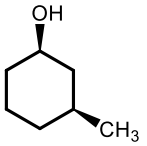


6-chloro-2-hexanol

B 



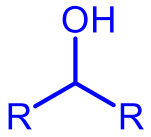
trans-4-methylcyclohexanol

C 

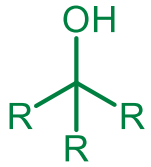
Notes

We learned to classify carbocations as methyl, primary (1°), etc. We can classify alcohols/alkyl halides similarly.

primary alcohol (1° alcohol)

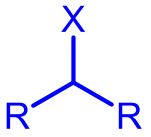


secondary alcohol (2° alcohol)

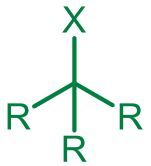


tertiary alcohol (3° alcohol)

primary alkyl halide (1°)



secondary alkyl halide (2°)



tertiary alkyl halide (3°)

These classifications are very important, because the different classes of alcohols and alkyl halides have different reactivities, as we will learn in detail later in the course.

Notes