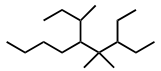
# Introduction to Alkane Nomenclature

http://masterorganicchemistry.com

## What's in a name?



3-ethyl-5-(1-methylpropyl)-4,4-dimethylnonane ← suffix

**the NUMBERS are called "locators"**
**items in BLUE are called "substituents".**
the name in **RED** at the end is called the **suffix.**

**The purpose of this sheet is to demonstrate the rules by which alkanes are named.**

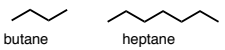
**ORDER OF BUSINESS**

**A. Determine the priority of functional groups (not covered here since we're dealing with alkanes only)**
**B. Find the longest linear chain of your molecule, or the largest ring** (whichever is greatest). This is the **Chain length rule** which defines both the "main chain" and also the suffix.
**-tiebreaker:** where more than one "path" along the molecule leads to the longest chain, **the main chain is the one that contains the most substituents.**
**C. Identify the substituents along your main chain.** Substituents are classified according to length of carbon chain and the suffix "yl" is attached.
**D.** Number your chain from one of the ends. The **LOWEST LOCATOR RULE** determines which end is chosen as carbon #1: **"Number the chain such as to provide the lowest possible locators for the chain."**
**-tiebreaker** for lowest-locator rule: **alphabetization**
**E. Multiple instances of substituents are given the prefixes di, tri, tetra, etc.**
**-note: must have locator for** all **substituents. Example:** 1,1-dimethyl is correct. 1-dimethyl is incorrect.
**F. Branched substituents are numbered and named seperately** from the main chain, and put in brackets.
**G. The FINAL name is assembled such as to arrange the substituents in alphabetical order.**
-"di", "tri", "tetra" are ignored for alphabetization purposes.
-prefixes like "n", "tert", "i" and "sec" are ignored for alphabetization purposes.
THE EXCEPTION is "isopropyl" and "isobutyl". For some reason these count as "i"
- not covered here, but this is also where one puts in descriptors like "cis", "trans", *(R), (S) (E), (Z)* and so on.

## Names for Hydrocarbon Chains and Rings

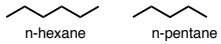
| | | | | |
|---|---|---|---|---|
| 1 | methane | | 3 | cyclopropane |
| 2 | ethane | | 4 | cyclobutane |
| 3 | propane | | 5 | cyclopentane |
| 4 | butane | | 6 | cyclohexane |
| 5 | pentane | | | |
| 6 | hexane | | | |
| 7 | heptane | | | |
| 8 | octane | | | |
| 9 | nonane | | | |
| 10 | decane | | | |
| 11 | undecane | | | |
| 12 | dodecane | | | |
| 20 | eicosane | | | |

7 and higher follow the same pattern.



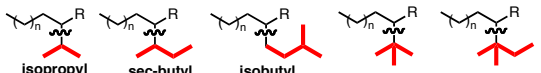
butane heptane

*Sometimes you will see "n" in front to indicate that it is a straight-chain alkane*



n-hexane n-pentane

**Trivial names for substituents**

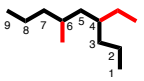


**isopropyl** **sec-butyl** **isobutyl** **tert-butyl** **tert-pentyl**

## A. Determining the Priority of Functional Groups.

*Too big a subject to cover on one sheet! This paper will focus on alkanes. Determining functional group priority will be the subject of a subsequent sheet.*

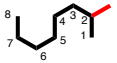
## B. Applying the Chain Length Rule



4-ethyl-6-methyl**nonane**

Longest chain is 9 carbons - suffix will be **nonane**

*Watch out! Longest chain might not be drawn as a "straight chain"*



2-methyl**octane**

*Longest chain is 8 carbons - suffix will be **octane***

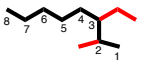
**Chains vs. rings**

Rings take priority over chains, assuming there are only alkyl groups in the chain. ***see note below

propyl**cyclobutane** butyl**cyclopropane**

**Tiebreaker: Alphabetization**

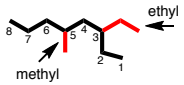
Where more than one "longest chain" exists, the more substituted chain is chosen as the "longest chain"



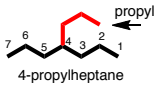
**3-ethyl-2-methyloctane**
(*NOT* - 3-isopropyloctane)

## C. Identifying Substituents

Substituents are carbon fragments branching off the main chain. They are named according to the number of carbons like the main chain would be, except the "ane" is dropped and replaced with "yl"




3-ethyl-5-methyloctane

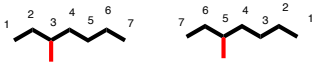



4-propylheptane

*** there seems to be some degree of confusion on this point. Both "1-butylcyclopropane" and "1-cyclopropylbutane" are commonly used. If someone can clarify, please write me.

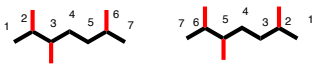
## D. Applying the Lowest Locator Rule

Number the chain from one end so as to provide the lowest locator possible for the first substituent.



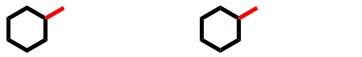
**3-methyl heptane** **NOT** *5-methyl heptane*

This also applies for *subsequent* substituents, if either direction would give the same number.



**2,3,6-trimethylheptane** **NOT** *2,5,6-trimethylheptane*

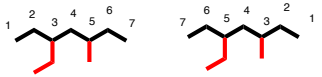
For rings with one substituent, the locator "1" can be dropped.



**methylcyclohexane** *the same as* **1-methylcyclohexane**

**Tiebreaker: Alphabetization**

If the same locators are obtained from either direction of the chain, the chain is numbered according to alphabetical order of the substituents.

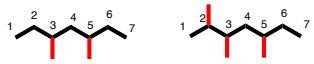


**3-ethyl-5-methylheptane** **NOT** **3-methyl-5-ethylheptane**

**1-ethyl-2-methylcyclobutane** **NOT** **1-methyl-2-ethylcyclobutane**

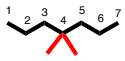
## E. Multiples of the Same Substituent

Multiples of the same substituent are given the prefixes "di", "tri", "tetra", etc. The lowest locator rule still applies.



**3,5-dimethylheptane** **2,3,5-trimethylheptane**

*Also applies to substituents on the same carbon:*



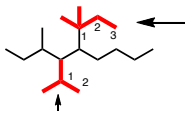
**4,4-dimethylheptane**

**NOT 4-dimethylheptane**
**NOT 4,4-methylheptane**

**Extremely common mistakes!**

## F. Dealing With Branched Substituents (the IUPAC Way)

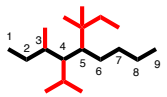
Treat each branched substituent as its own naming problem.
Carbon #1 of the branched substituent will be where it meets the main chain.



•Longest chain is propyl
•Methyl substituents are on carbon #1
•Name of substituent is (**1,1-dimethylpropane**)

•Longest chain is ethyl
•Methyl substituent is on carbon #1
•Name of substituent is (**1-methylethyl**)

**We put the name in brackets to avoid confusing the numbers of the branched substituent with the numbers of the main chain.**



**3-methyl 4-(1-methylethyl) 5-(1,1-dimethylpropyl) nonane**

In certain instances, you may see the trivial names isopropyl, isobutyl, tert-butyl, tert-pentyl used.

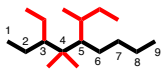
**e.g. 4-isopropyl-3-methyl-5-tert-pentylnonane.**

The official IUPAC nomenclature system will never let you down. It would probably be best to just go with that.

## G. Putting the Name Together.

1. Put your substituents together in **alphabetical order.**
   For alphabetization purposes:
   **IGNORE** •"di", "tri", "tet", etc.
   • *sec-, tert-, n-,*
   •cyclo-

   **DO NOT IGNORE**
   **• "iso". For some strange reason "isopropyl" is alphabetized under "i" and not "p". Don't ask me why.**
2. Affix the **locators.**
3. Make sure any **branched substituents** are in brackets.
4. Attach the **suffix** at the end.



**3-ethyl-5-(1-methylpropyl)-4,4-dimethylnonane**



Errors/omissions/suggestions?
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For more comoplete resources on nomenclature consult:
1) "Organic Chemistry Online" by William Reusch: http://www2.chemistry.msu.edu:80/faculty/reusch/VirtTxtJml/intro1.htm
2) IUPAC "Blue Book" http://www.acdlabs.com/iupac/nomenclature/