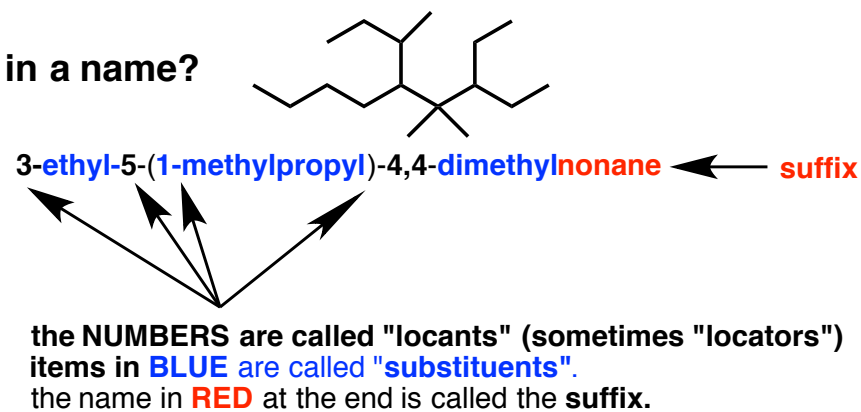


Introduction to Alkane Nomenclature

<http://masterorganicchemistry.com>

What's in a name?



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: 2,2-dimethyl is correct. 2-dimethyl is incorrect.

F. Branched substituents are numbered and named separately 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.

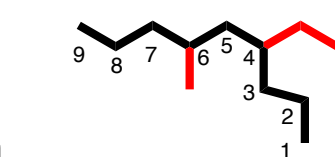
THE EXCEPTION is "isopropyl" and "isobutyl". For some reason these count as "i"

- not covered here, but this is also where one puts in descriptors like "cis", "trans", (R), (S) (E), (Z) and so on.

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.

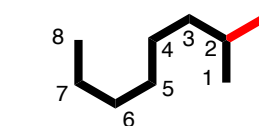
B. Applying the Chain Length Rule



4-ethyl-6-methylnonane

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

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



2-methyloctane

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

Chains vs. rings

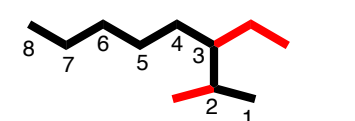
Rings take priority over chains, assuming there are only alkyl groups in the chain. ***see note below



propyl**cyclobutane** cyclopropyl**butane**

Tiebreaker: Alphabetization

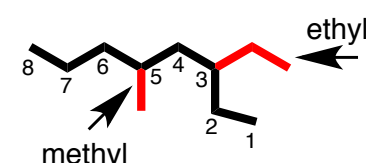
Where more than one "longest chain" exists, the more substituted chain is chosen as the "longest chain"



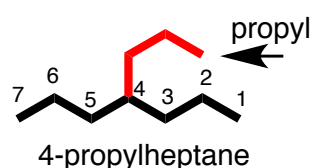
3-ethyl-2-methyloctane
(NOT - 3-isopropyloctane)

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"



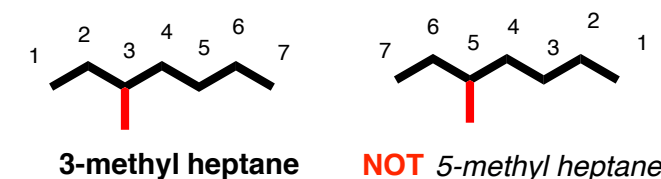
3-ethyl-5-methyloctane



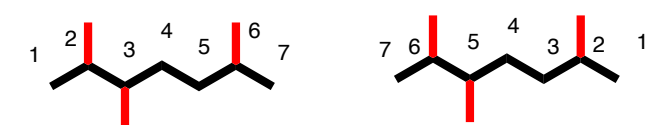
4-propylheptane

D. Applying the Lowest Locator Rule

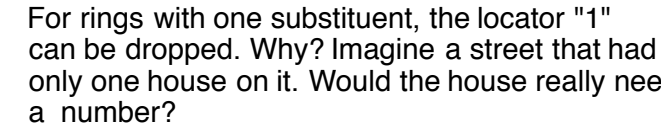
Number the chain from one end so as to provide the lowest locator possible for the first substituent.



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



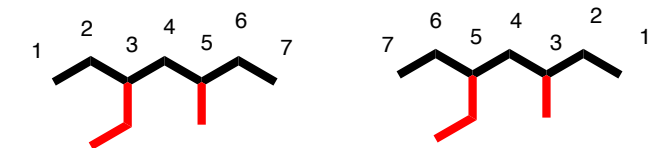
For rings with one substituent, the locator "1" can be dropped. Why? Imagine a street that had only one house on it. Would the house really need a number?



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.



Also applies to substituents on the same carbon:



4,4-dimethylheptane

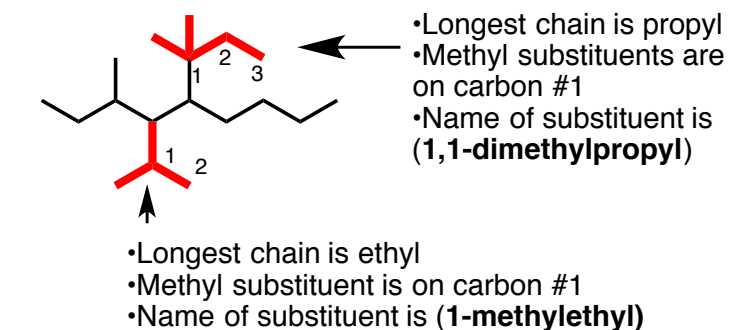
NOT 4-dimethylheptane
NOT 4,4-methylheptane

Extremely common mistakes!

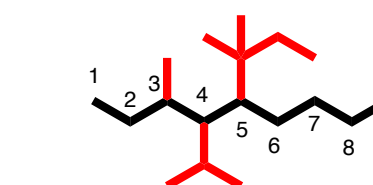
F. Dealing With Branched Substituents (the IUPAC Way)

Treat each branched substituent as its own naming problem.

Carbon #1 of the branched substituent will be where it meets the main chain.



We put the name in parentheses 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-

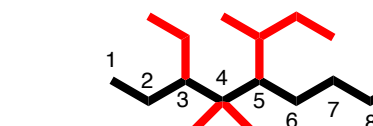
DO NOT IGNORE

• "iso". For some reason "isopropyl" is alphabetized under "i" and not "p".

2. Affix the locators.

3. Make sure any **branched substituents** are in parentheses

4. Attach the **suffix** at the end.

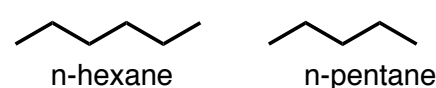


3-ethyl-4,4-dimethyl-5-(1-methylpropyl)-nonane

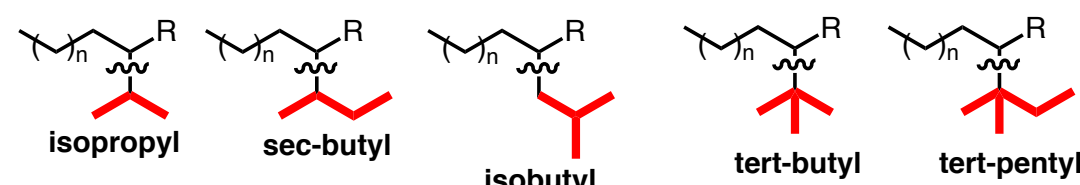
Names for Hydrocarbon Chains and Rings

1	methane		3	cyclopropane
2	ethane		4	cyclobutane
3	propane		5	cyclopentane
4	butane		6	cyclohexane
5	pentane		7 and higher follow the same pattern.	
6	hexane			
7	heptane			
8	octane			
9	nonane			
10	decane			
11	undecane			
12	dodecane			
20	eicosane			

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



Trivial names for substituents



*** IUPAC 61.2 says, "Choice between these methods [either choosing rings or chains as the root] is made according to the more appropriate of the following principles: (a) the maximum number of substitutions into a single unit of structure; (b) treatment of a smaller of structure as a substituent into a larger."

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<http://masterorganicchemistry.com>

Errors/omissions/suggestions?
james@masterorganicchemistry.com

For more complete 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/>