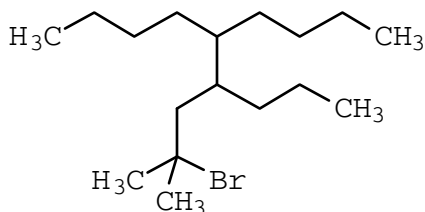


## CH203 Handout

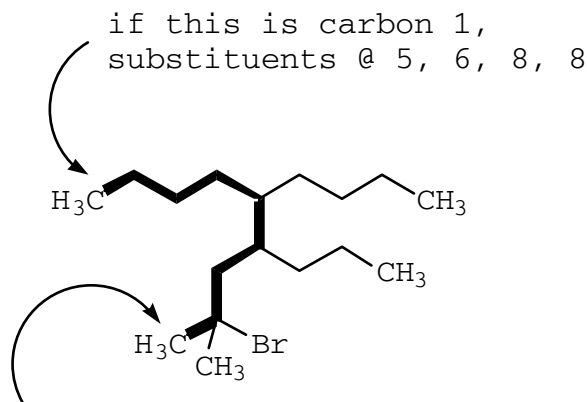
### Alkanes: Naming and Assigning Position numbers to Substituents

- Begin numbering carbons in the parent from an end of the chain
- Consider different numbering systems: choose the numbering system that gives the lowest number to a substituent at the first point of difference in the numbering systems
- Equivalent substituent numbering systems? – Choose the numbering system that gives the lowest number to the substituent that is first alphabetically

Example First, find the parent chain in the molecule shown below. Then, assign position numbers to its substituents.



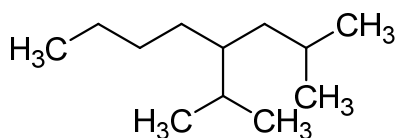
Solution We consider starting numbering the carbons from both ends of the parent chain. We prefer the numbering scheme that assigns the lowest number to a substituent at the first point of difference in the numbering systems.



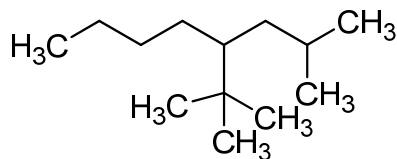
if this is carbon 1,  
substituents @ 5, 6, 8, 8

if this is carbon 1,  
substituents @ 2, 2, 4, 5;  
**this one wins**  
**because 2 is lower than 5**

- The prefix *iso* is written with no hyphen and is treated during alphabetical priority assignment.
  - The prefixes *sec-* and *tert-* are written with a hyphen and not treated during alphabetical priority assignment.
- Please consider ~see page 89 of text for discussion

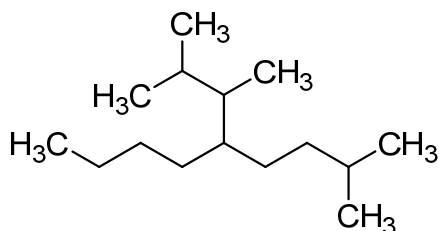


4-isopropyl-2-methyloctane

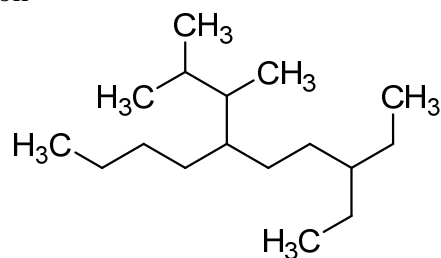


4-*tert*-butyl-2-methyloctane

- For alphabetization of more formal naming, consider *di*, and *tri* prefixes when assigning order priority.
- Please consider: see page 89 of text for discussion

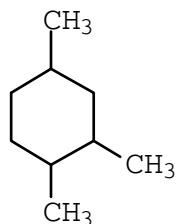


5-(1,2-Dimethylpropyl)-2-methylnonane



3-ethyl-6-(1,2-dimethylpropyl)-decane

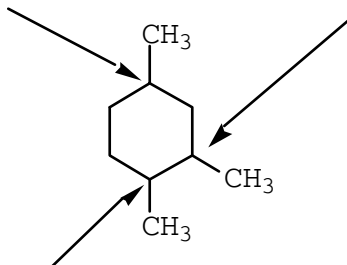
Example Assign position numbers to the substituents in this molecule.



Solution The parent is cyclohexane. Again, we consider different numbering schemes and prefer the numbering scheme that assigns the lowest number to a substituent at the first point of difference in the numbering systems.

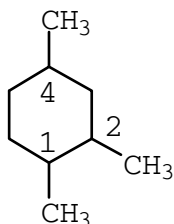
if this is carbon 1  
and you number clockwise,  
substituents @ 1, 3, 4;  
if you number anticlockwise,  
substituents @ 1, 4, 5

if this is carbon 1  
and you number clockwise,  
substituents @ 1, 2, 5;  
if you number anticlockwise,  
substituents @ 1, 3, 6



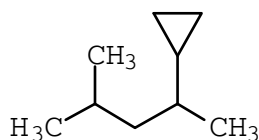
if this is carbon 1  
and you number clockwise,  
substituents @ 1, 4, 6;  
if you number anticlockwise,  
substituents @ 1, 2, 4

All of the numbering systems have a “1” as the first number: no decision can be made so we look at the second number. Two of the numbering systems have a “2” as the second number, but still no decision can be made. Look at the third number: “1, 2, 4” wins out over “1, 2, 5” because “4” is lower than “5”. The correct numbering is

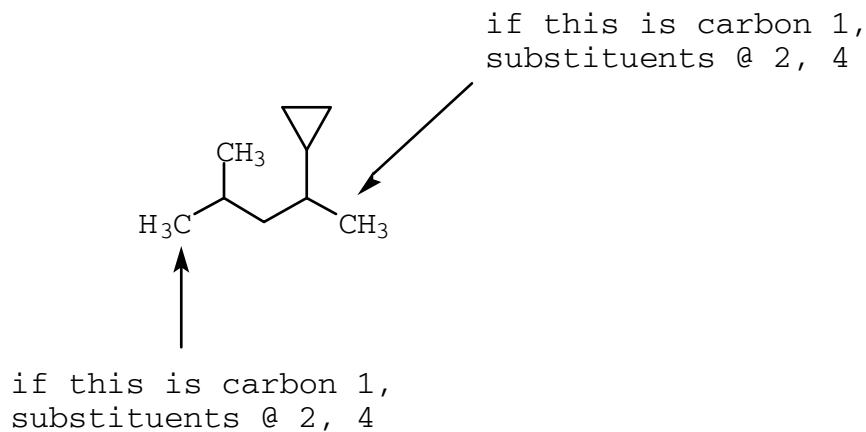


*The correct name of this compound is 1,2,4-trimethylcyclohexane*

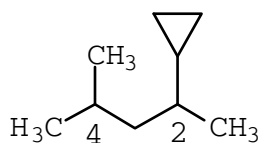
Example Assign position numbers to the substituents in this molecule.



Solution The parent is pentane. Both numbering schemes yield substituents at 2 and 4:



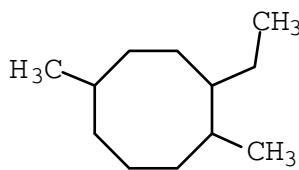
To break the tie, we note that “cyclopropyl” is alphabetized before “methyl”. The preferred numbering gives the lowest number to the substituent that is alphabetically first, but this rule is used only as a tie-breaker! The correct numbering is



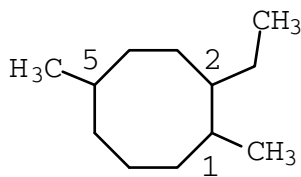
Formulating systematic names: Putting it all together

- List substituents with their position numbers alphabetically
- Indicate the number of identical substituents by using replicating prefixes (i.e., di, tri, tetra, etc.)
- Ignore replicating prefixes when alphabetizing; for example, triethyl comes before methyl because “e” comes before “m” -- we simply pretend that the “tri” is not there
- “Cyclo” is not a replicating prefix -- don’t ignore it

Problem Write the systematic name.



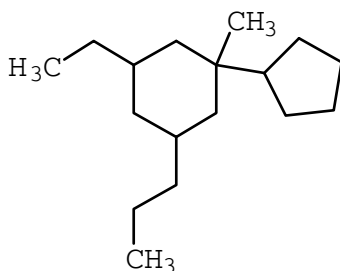
Solution The parent is cyclooctane. The correct numbering is



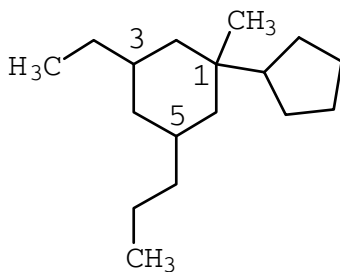
The name is 2-ethyl-1,5-dimethylcyclooctane. Several features worth noting:

- “ethyl” comes before “methyl”, so “ethyl” is written first -- we pretend that the “di” in “dimethyl” is not there
- hyphens set off numbers from words
- commas separate numbers
- all systematic names, except those of carboxylic acids and of esters are one-word names, sort of like Madonna, Cher and Nelly

Problem Write the systematic name.



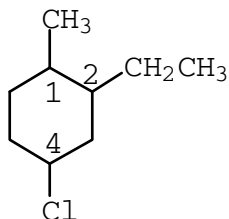
Solution The parent is cyclohexane because the six-carbon ring is larger than the five-carbon ring. The correct numbering is



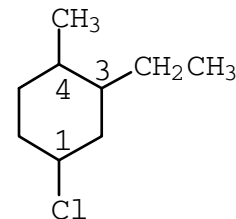
If we number from carbon 1 clockwise, we get substituents at 1, 1, 3, and 5. If we number from carbon 1 anticlockwise, we get substituents at 1, 1, 3, and 5. We have a tie in the numbering systems so we prefer the numbering that gives the lowest number to the substituent that is first alphabetically: 3-ethyl is preferred over 3-propyl. The name is 1-cyclopentyl-3-ethyl-1-methyl-5-propylcyclohexane.

*Additional Examples*

1)

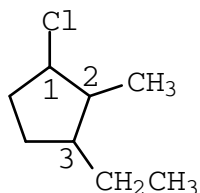


The 1,2,4 numbering wins out over the 1,3,4 numbering because  $2 < 3$

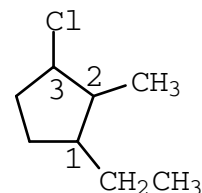


The correct name of the compound is 4-chloro-2-ethyl-1-methylcyclohexane  
(*not* 1-chloro-3-ethyl-4-methylcyclohexane)

2)

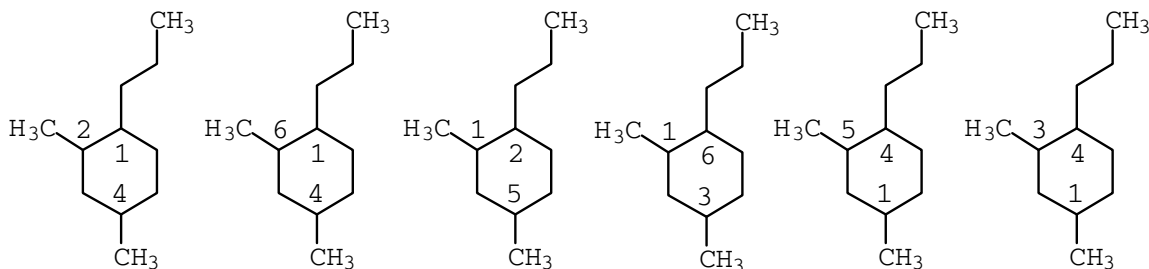


Both numbering systems are 1,2,3: break the tie by assigning the lowest number to the substituent that is first alphabetically



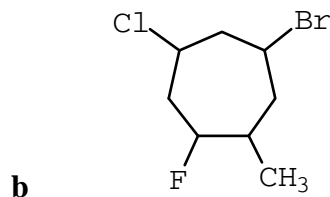
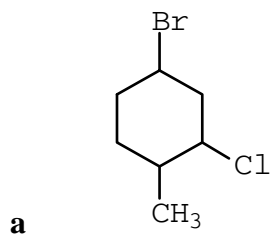
The correct name of the compound is 1-chloro-3-ethyl-2-methylcyclopentane

3) Consider the numbering systems of the compound below:



All the numbering systems have a “1” as the first number. Look at the second number: the numbering systems that have a “2” as the second number (1,2,4 and 1,2,5) win out over all the remaining systems. “1,2,4” is the overall winner because  $4 < 5$ .

*Additional Practice problems:* Provide the name for the following cycloalkanes:



- a** 4-bromo-2-chloro-1-methylcyclohexane  
**b** 4-bromo-6-chloro-1-fluoro-2-methylcycloheptane