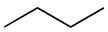
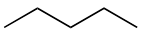
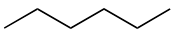
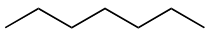
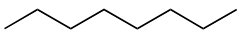
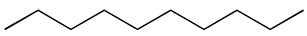
Basic IUPAC Nomenclature I

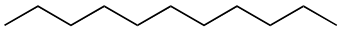
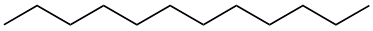
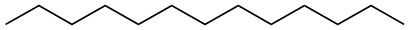
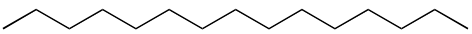
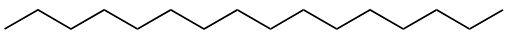
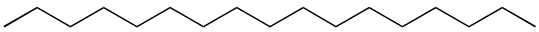
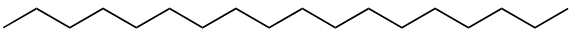
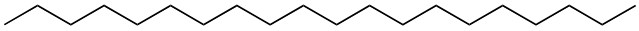
Straight Chain Alkanes

- Straight chain alkanes have only carbon and hydrogen atoms.
- Formula is $C_xH_{(2x+2)}$
- All the carbons in alkanes are sp^3 hybridized and in straight chain alkanes all the carbons are linked in a straight line. (Exactly two ends)
- Straight chain alkanes are named for the number of carbons in the chain.
- All straight chain alkane names end in –ane; which shows that the only functional group present is alkanes.

Basic Straight Chain Alkanes C_1 - C_{10}

C_1 **methane**	CH_4	CH_4
C_2 **ethane**	CH_3CH_3	
C_3 **propane**	$CH_3CH_2CH_3$	
C_4 **butane**	$CH_3(CH_2)_2CH_3$	
C_5 **pentane**	$CH_3(CH_2)_3CH_3$	
C_6 **hexane**	$CH_3(CH_2)_4CH_3$	
C_7 **heptane**	$CH_3(CH_2)_5CH_3$	
C_8 **octane**	$CH_3(CH_2)_6CH_3$	
C_9 **nonane**	$CH_3(CH_2)_7CH_3$	
C_{10} **decane**	$CH_3(CH_2)_8CH_3$	

Advanced Straight Chain Alkanes $C_{11} – C_{20}$

C_{11} **undecane**	$CH_3(CH_2)_9CH_3$	
C_{12} **dodecane**	$CH_3(CH_2)_{10}CH_3$	
C_{13} **tridecane**	$CH_3(CH_2)_{11}CH_3$	
C_{14} **tetradecane**	$CH_3(CH_2)_{12}CH_3$	
C_{15} **pentadecane**	$CH_3(CH_2)_{13}CH_3$	
C_{16} **hexadecane**	$CH_3(CH_2)_{14}CH_3$	
C_{17} **heptadecane**	$CH_3(CH_2)_{15}CH_3$	
C_{18} **octadecane**	$CH_3(CH_2)_{16}CH_3$	
C_{19} **nonadecane**	$CH_3(CH_2)_{17}CH_3$	
C_{20} **icosane**	$CH_3(CH_2)_{18}CH_3$	

Notes:

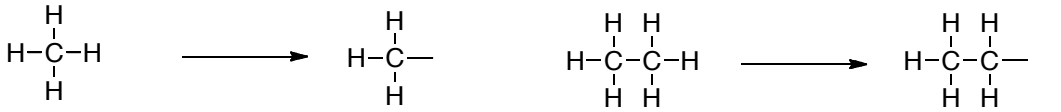
- With 5 or more carbons straight chain alkanes count generally using Greek prefixes.
- Memorizing 1-10 is sufficient for 8A, students in 118A should know 1-20.

Basic IUPAC Nomenclature II

Alkyl Groups

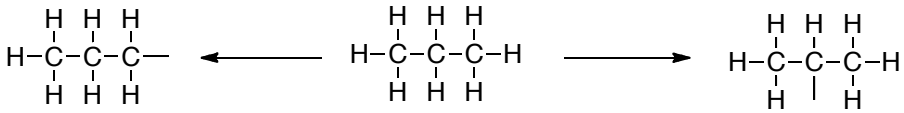
- You can make an alkane into an alkyl group by removing a hydrogen.

- Alkyl groups of straight chains are named by dropping the ending –ane and adding the ending –yl to the base name of the chain.



a **methane** molecule — a **methyl** group — an **ethane** molecule — an **ethyl** group

- Once we get to three or more carbons there are choices. We can form straight chain or branched alkyl groups.



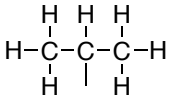
a **propyl** group
a straight chain or n-alkyl substituent

a **propane** molecule

an **isopropyl** group
a branched chain substituent

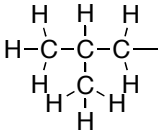
- Many smaller branched alkyl groups get common names. These names are old fashioned, but are still often used. The following common names are in general use and should be remembered.

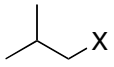
isopropyl



the iso- prefix is included in alphabetization

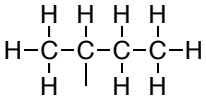
isobutyl

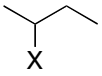




the iso- prefix is included in alphabetization

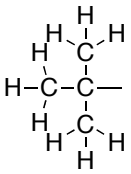
***sec*-butyl**





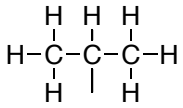
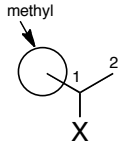
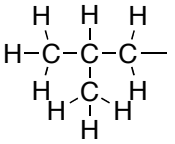
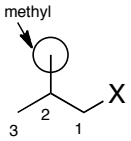
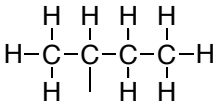
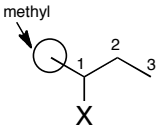
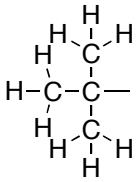
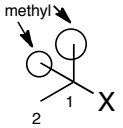
the *sec*- prefix is italicized and separate from the name and is NOT included in alphabetization.

***tert*-butyl**



the *tert*- prefix is italicized and separate from the name and is NOT included in alphabetization.

- Branched alkyl groups can also be named by IUPAC by treating each branch as a substituent off the main chain. When naming branched alkyl groups using IUPAC the carbon attached to the point of interest (e.g. main chain) is carbon one.

Common		IUPAC
isopropyl	 	**1-methylethyl**
isobutyl	 	**2-methylpropyl**
***sec*-butyl**	 	**1-methylpropyl**
***tert*-butyl**	 	**1,1-dimethylethyl** *

* Unlike most prefixes di-, tri-, tetra- etc prefixes in branched substituents count towards alphabetical order. e.g., 1,1-**D**imethylethyl rather than 1,1-di**M**ethylethyl.

Notes:

- Alkyl groups are generally substituents meaning they have a bond attached to something of note (e.g., halogens, amines, alcohols, ethers, longer chains).
- Alkyl groups are never complete molecules on their own.
- The variable –R represents any alkyl group.
- **iso**- groups generally have the form $(CH_3)_2CH$-X
- ***sec-*** groups attach via a secondary carbon
- ***tert-*** groups attach via a tertiary carbon

Basic IUPAC Nomenclature III

Branched Chain Alkanes/Haloalkanes

- Branched chain alkanes have only carbon and hydrogen atoms. haloalkanes have a halogen (F, Cl, Br, I)

- Formulas are $C_nH_{(2n+2)}$ for alkanes or $C_nH_{(2n+2-y)}X_y$ for haloalkanes

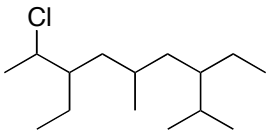
- All the carbons in alkanes are sp^3 hybridized and in branched chain alkanes the chain forks. (More than two ends)

- IUPAC Nomenclature of *branched alkanes* follows these steps:
  1) Find the longest chain of continuous **carbons**. This is now the main chain. Name this chain as if it were a straight chain alkane.
     a. If two chains are the same length choose the one with more branches.
  2) Count the carbons in the main chain left to right and right to left. The direction you *first* run into a substituent is the direction use to number the chain.
     a. If the numbers are the same go to the next nearest substituent
     b. If the numbers are exactly the same regardless of direction the lower numbers go to the first substituent in alphabetical order.
  3) Give each substituent a number according to which carbon it's attached to.
  4) List the substituents in alphabetical order in front of the main chain.
     a. Branched substituents get parenthesis around them
     b. Numbers are separated from numbers by commas
     c. Numbers are separated from words by hyphens
  5) Multiple straight chain substituents of the same kind are combined and given a prefix to indicate the number (di-, tri-, tetra-). These prefixes do not count towards alphabetical order. If the substituent is branched (bis-, tris-, tetrakis-) are used.

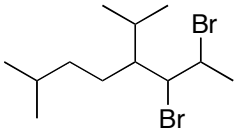
Notes:

- Sometimes it helps to think of each carbon in the main chain as a house on a street. The substituents that live there each get an address (number) according to which house (carbon) they live at.
- Once you've found your main chain circling or labeling it can show you what you still have left to name as substituents
- To find the longest chain pick an end and follow it to the first branch. Make sure you have the longest end on that branch. Follow the chain to the next branch selecting the longest continuing chain each time you find a branch until you run out of molecule.
- F- is Fluoro, Cl- is Chloro, Br- is Bromo, I- is Iodo. They get no special priority

Examples:

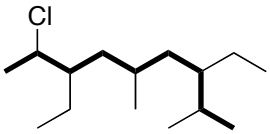


Compound A



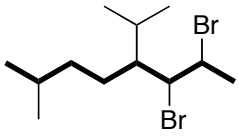
Compound B

1)



a **nonane**

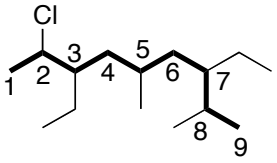
We could have started in the lower left or ended in the upper right and gotten the same length, but this chain has 5 substituents rather than 3 or 4.



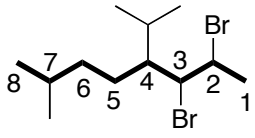
an **octane**

We could start at the lower left methyl and the result would be exactly the same.

2)

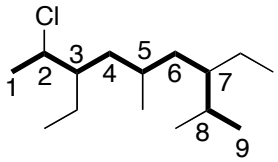


Left to right we get substituents at positions 2,3,5,7,and 8
Right to left we also get substituents at postions 2,3,5,7, and 8.
The first substituent L-->R is **C**hloro, the first substituent R-->L is **M**ethyl.
C comes first so L-->R is correct.

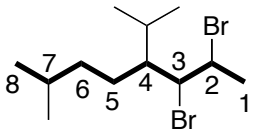


Left to right we get substituents at positions 2, **5**, 6, and 7.
Right to left we also get substituents at postions 2,**3**,4, and 7.
2 = 2 so we go on to the next substituent and **3 < 5** so we use R--> L

3)



2-chloro
3-ethyl
5-methyl
7-ethyl
8-methyl



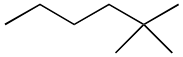
2-bromo
3-bromo
4-isopropyl or 4-(1-methylethyl)
7-methyl

4,5)

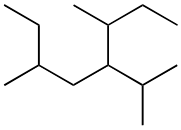
2-chloro-3,7-diethyl-5,8-methylnonane

2,3-dibromo-4-isopropyl-7-methyloctane
or
2,3-dibromo-7-methyl-4-(1-methylethyl)octane

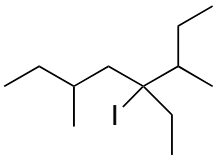
Practice Alkane and Haloalkane Nomenclature:



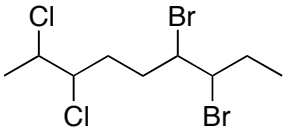
Compound A



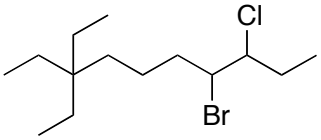
Compound B



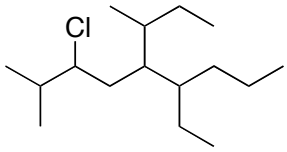
Compound C



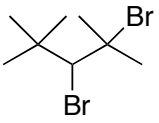
Compound D



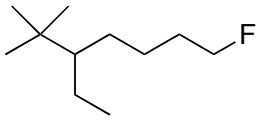
Compound E



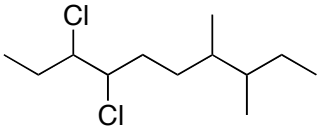
Compound F



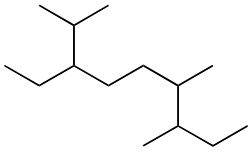
Compound G



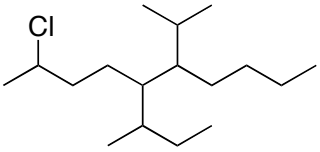
Compound H



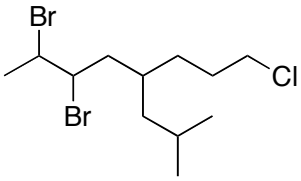
Compound I



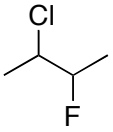
Compound J



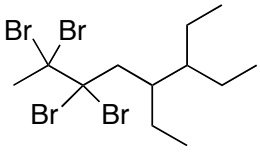
Compound K



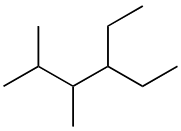
Compound L



Compound M



Compound N



Compound O

Practice Alkane and Haloalkane Nomenclature Key:

Compound A: 2,2-dimethylhexane

Compound B: 4-isopropyl-3,6-dimethyloctane or
3,6-dimethyl-4-(1-methylethyl)octane

Compound C: 4-ethyl-4-iodo-3,6-dimethyloctane

Compound D: 6,7-dibromo-2,3-dichlorononane

Compound E: 7-bromo-8-chloro-3,3-diethyldecane

Compound F; 5-*sec*-butyl-3-chloro-6-ethyl-2-methylnonane or
3-chloro-6-ethyl-2-methyl-5-(1-methylpropyl)nonane

Compound G: 2,3-dibromo-2,4,4-trimethylpentane

Compound H: 5-ethyl-1-fluoro-6,6-dimethylheptane

Compound I: 3,4-dichloro-7,8-dimethyldecane

Compound J: 3-ethyl-2,6,7-trimethylnonane

Compound K: 5-*sec*-butyl-2-chloro-6-isopropyldecane or
2-chloro-6-(1-methylethyl)-5-(1-methylpropyl)decane

Compound L: 6,7-dibromo-1-chloro-4-isobutyloctane or
6,7-dibromo-1-chloro-4-(2-methylpropyl)octane

Compound M: 2-chloro-3-fluorobutane

Compound N: 2,2,3,3-tetrabromo-5,6-diethyloctane

Compound O: 4-ethyl-2,3-dimethylhexane

Basic IUPAC Nomenclature IV

Cycloalkanes

- Cycloalkanes have only carbon and hydrogen atoms.

- Formulas are $C_nH_{(2n)}$

- All the carbons in alkanes are sp^3 hybridized and in a cycloalkane a ring is formed. (No ends)

- Cycloalkanes can be substituted like regular alkanes

- IUPAC Nomenclature of *cycloalkanes* follows these steps:
  1) Find the ring. This is now the main chain. Count the carbons and name chain as if it were a straight chain alkane. Add the prefix cyclo- to the name to get the full base name of the ring.
  2) If there are substituents:
     a. 1 substituent → the carbon the substituent is attached to is carbon-1. There is no need to number the substituent.
     b. 2 substituents → the substituents will have the same numbers, so the first in alphabetical order will be at carbon-1. Substituents should be numbered.
     c. 3 or more substituents → Number substituents so that the lowest possible numbers are used. If there is a tie use alphabetical order.
  3) Give each substituent a number according to which carbon it's attached to.
  4) List the substituents in alphabetical order in front of the main chain.
     a. Branched substituents get parenthesis around them
     b. Numbers are separated from numbers by commas
     c. Numbers are separated from words by hyphens
  5) Multiple straight chain substituents of the same kind are combined and given a prefix to indicate the number (di-, tri-, tetra-). These prefixes do not count towards alphabetical order. If the substituent is branched (bis-, tris-, tetrakis-) are used.
  6) Indicate stereochemistry using *cis-* or *trans-* prefixes for disubstituted rings or *R,S* labels for multiply substituted rings.

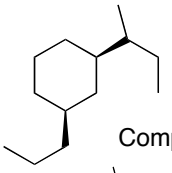
Notes:

- Cycloalkanes can become cycloalkyl substituents

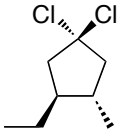
- Two substituents on the same carbon are almost always 1,1-disubstituted.

- *Cis*-substituents are on the same side and sound similar, *trans*-substituents are on opposite sides and you have to go across the ring.

Examples:

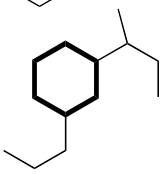


Compound C

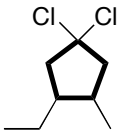


Compound D

1)

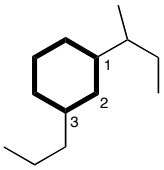


a **cyclohexane**

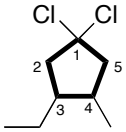


a **cyclopentane**

2)

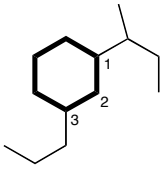


butyl comes before propyl
and 1,3 is lower than 1, 5

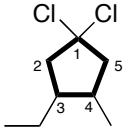


1, 1, 3, 4 is lower than 1, 2, 4, 4
(1,1 always wins)
ethyl comes before methyl so we
go counterclockwise

3)



1-*sec*-butyl or 1-methylpropyl
3-propyl



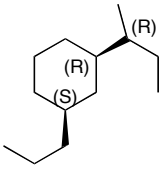
1-chloro
1-chloro
3-ethyl
4-methyl

4,5)

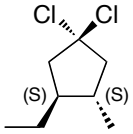
1-*sec*-butyl-3-propylcyclohexane
or
1-(1'-methylpropyl)-3-propylcyclohexane

1,1-dichloro-3-ethyl-4-methylcyclopentane

6)



same side = **cis**

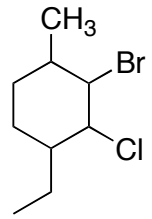


ethyl = #1 CH, #2 CH_2CCl_2, #3 CH_2CH_3, #4 H
= *S*
methyl = #1 CH, #2 CH_2CCl_2, #3 CH_3, #4 H
= *S*

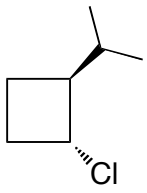
cis-1-*sec*-butyl-3-propylcyclohexane
or
cis-1-(1'-methylpropyl)-3-propylcyclohexane

(3S,4S)-1,1-dichloro-3-ethyl-4-methylcyclopentane

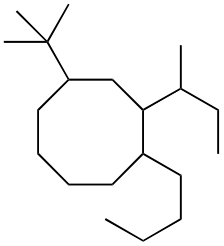
Practice Cycloalkane Nomenclature:



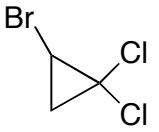
Compound A



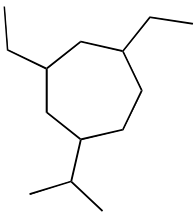
Compound B



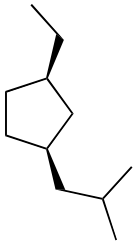
Compound C



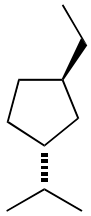
Compound D



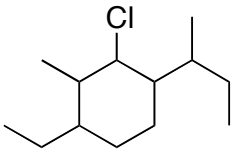
Compound E



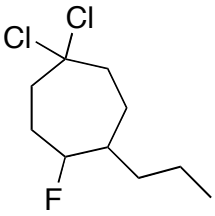
Compound F



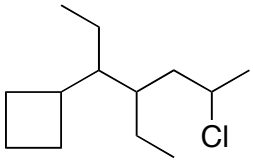
Compound G



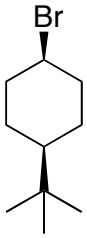
Compound H



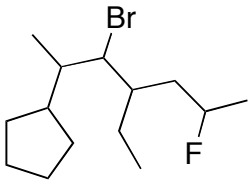
Compound I



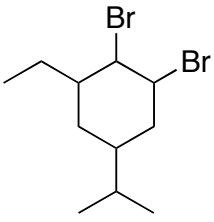
Compound J



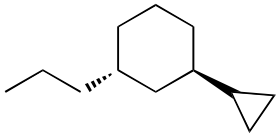
Compound K



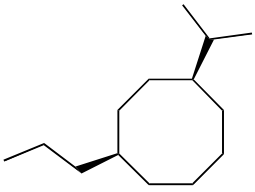
Compound L



Compound M



Compound N



Compound O

Practice Cycloalkane Nomenclature Key:

Compound A: 3-bromo-2-chloro-1-ethyl-4-methylcyclohexane

Compound B: *trans*-1-chloro-2-isopropylcyclobutane or
trans-1-chloro-2-(1-methylethyl)cyclobutane or
(1R,2S)-1-chloro-2-(1-methylethyl)cyclobutane

Compound C: 1-butyl-2-*sec*-butyl-4-*tert*-butylcyclooctane or
1-butyl-4-(1,1-dimethylethyl)-2-(1-methylpropyl)cyclooctane

Compound D: 2-bromo-1,1-dichlorocyclopropane

Compound E: 1,3-diethyl-5-isopropylcycloheptane or
1,3-diethyl-5-(1-methylethyl)cycloheptane

Compound F: *cis*-1-ethyl-3-isobutylcyclopentane or
cis-1-ethyl-3-(2-methypropyl)cyclopentane or
(1R,3R)-1-ethyl-3-(2-methypropyl)cyclopentane

Compound G: *trans*-1-ethyl-3-isopropylcyclopentane or
trans-1-ethyl-3-(1-methyethyl)cyclopentane or
(1R,3R)-1-ethyl-3-(1-methyethyl)cyclopentane

Compound H: 1-*sec*-butyl-2-chloro-4-ethyl-3-methylcyclohexane or
3-chloro-1-ethyl-2-methyl-4-(1-methylpropyl)cyclohexane

Compound I: 1,1-dichloro-4-fluoro-5-propylcycloheptane

Compound J: 2-chloro-5-cyclobutyl-4-ethylheptane

Compound K: *cis*-1-bromo-4-*tert*-butylcyclohexane or
cis-1-bromo-4-(1,1-dimethylethyl)cyclohexane

Compound L: 3-bromo-2-cyclopentyl-4-ethyl-6-fluoroheptane

Compound M: 1,2-dibromo-3-ethyl-5-isopropylcyclohexane or
1,2-dibromo-3-ethyl-5-(1-methylethyl)cyclohexane

Compound N: *trans*-1-cyclopropyl-3-propylcyclohexane or
(1R,3R)-1-cyclopropyl-3-propylcyclohexane

Compound O: *cis*-1-isopropyl-4-propylcyclooctane
cis-1-(1-methylethyl)-4-propylcyclooctane
(1S,4R)-1-(1-methylethyl)-4-propylcyclooctane