Alkanes

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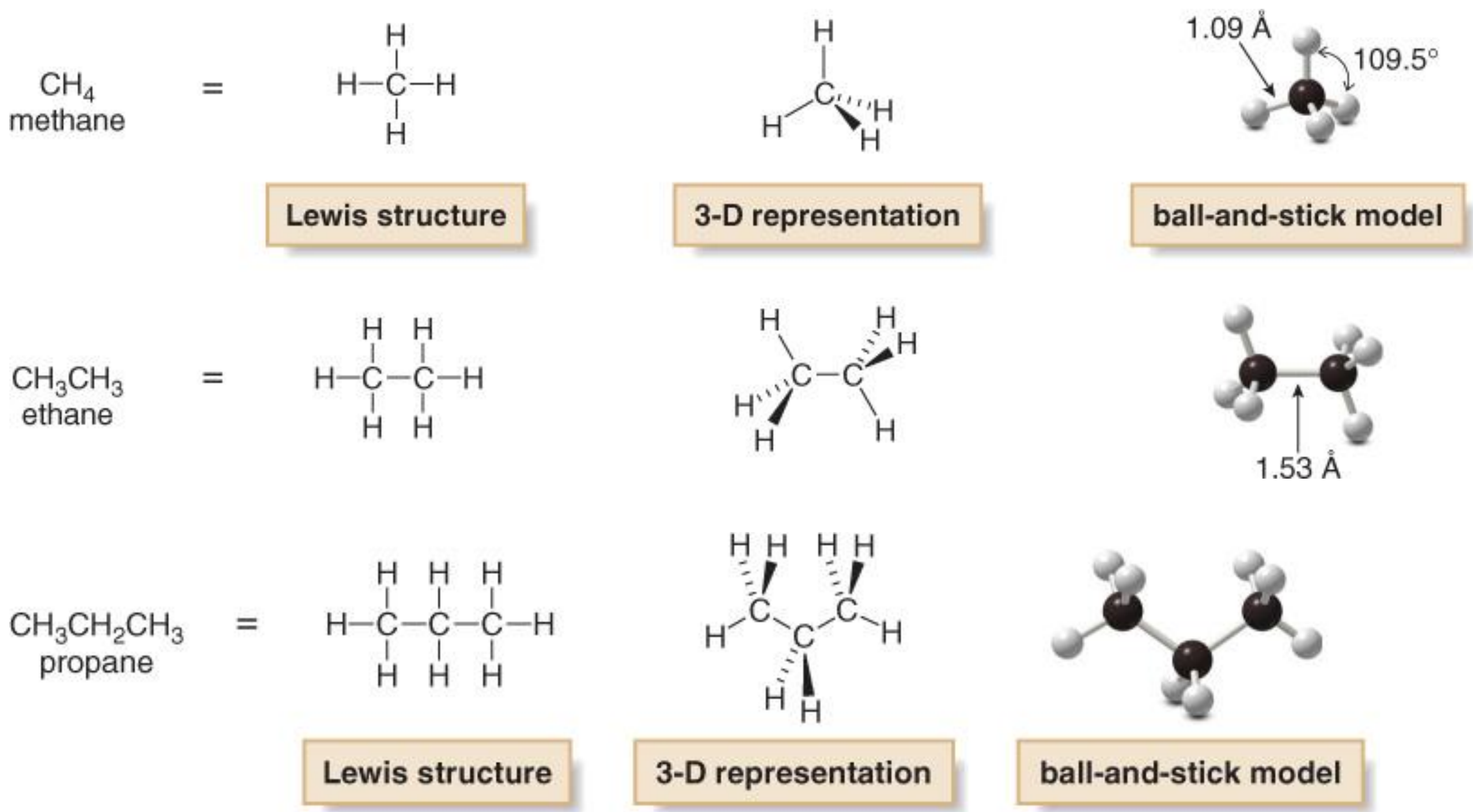
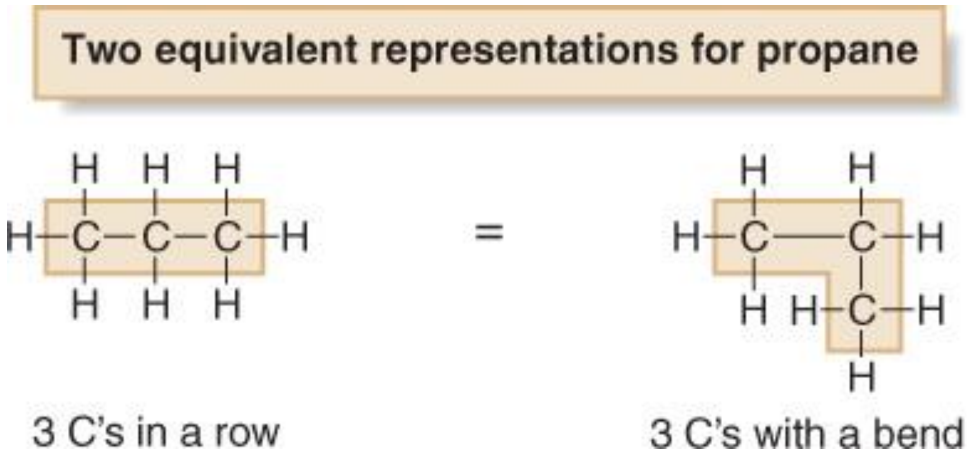
Alkanes

- aliphatic hydrocarbons having C—C and C—H σ bonds.
- Acyclic alkanes
  - molecular formula C_nH_{2n+2}
  - contain only linear and branched chains of carbon atoms.
  - Saturated hydrocarbons -- have the maximum number of hydrogen atoms per carbon.
- Cycloalkanes
  - carbons joined in one or more rings.
  - molecular formula C_nH_{2n}
    - have two fewer H atoms than an acyclic alkane with the same number of carbons.

- All C atoms in an alkane are surrounded by four groups
- *sp*^{3} hybridized
- Tetrahedral (all bond angles are 109.5^0)

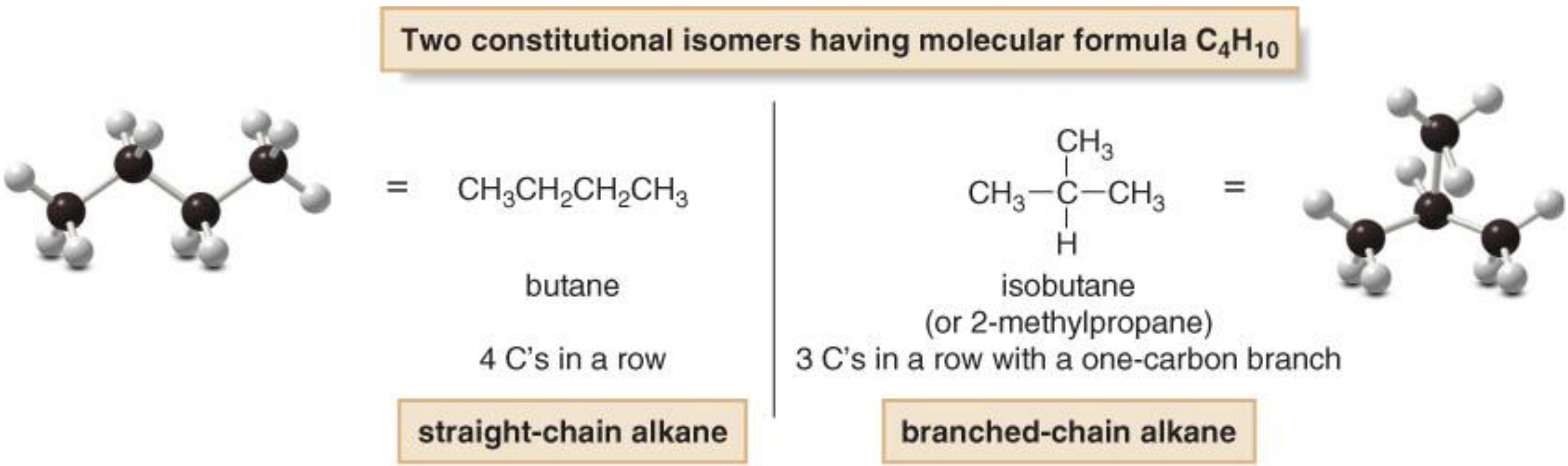


- In propane and higher molecular weight alkanes, the carbon skeleton can be drawn in a variety of ways and still represent the same molecule.



In a Lewis structure, the bends in a carbon chain don't matter.

There are two different ways to arrange four carbons, giving two compounds with molecular formula C_4H_{10}.

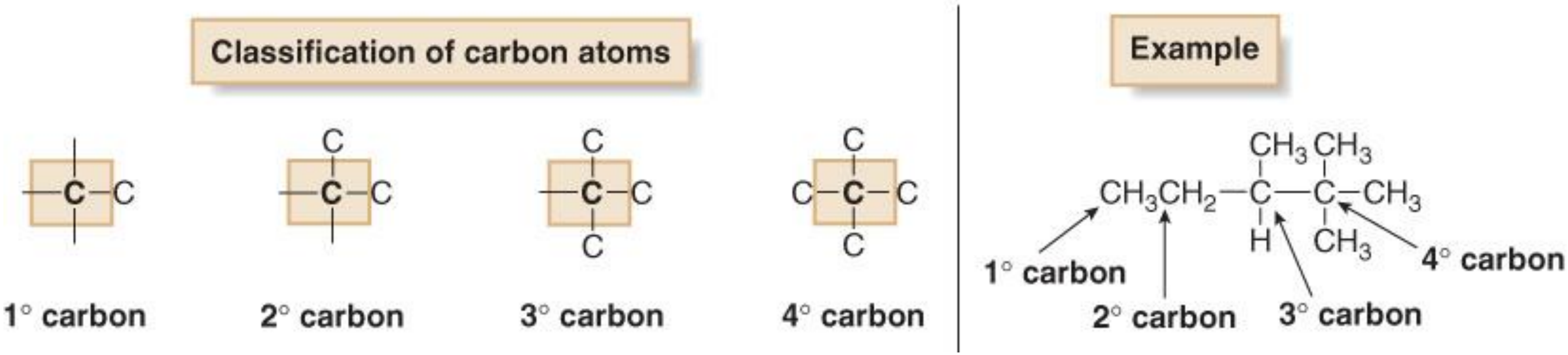


Butane and isobutane are constitutional isomers (different compounds with the same molecular formula.)

Constitutional isomers differ in the way the atoms are connected to each other.

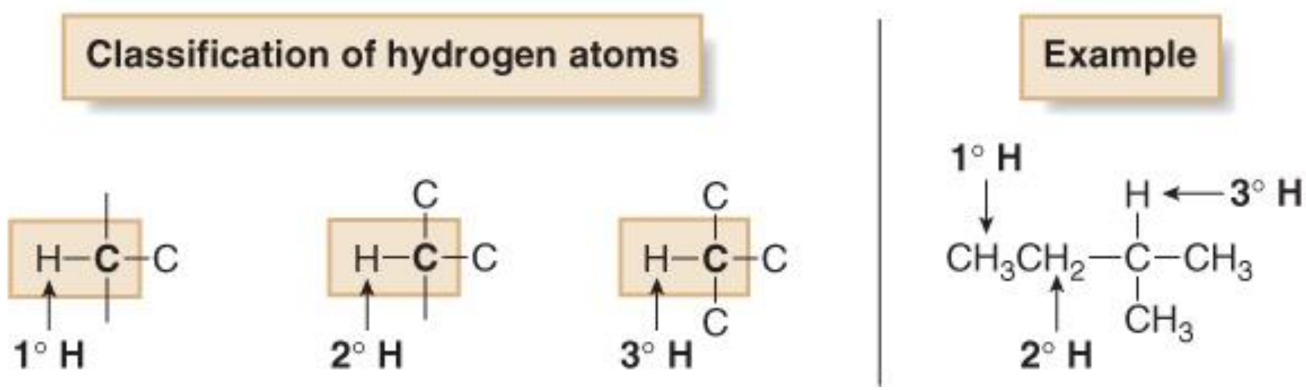
Carbon atoms in alkanes and other organic compounds are classified by the number of other carbons directly bonded to them.

- A *primary carbon* (1° carbon) is bonded to *one* other C atom.
- A *secondary carbon* (2° carbon) is bonded to *two* other C atoms.
- A *tertiary carbon* (3° carbon) is bonded to *three* other C atoms.
- A *quaternary carbon* (4° carbon) is bonded to *four* other C atoms.



Hydrogen atoms are classified as primary (1^0), secondary (2^0), or tertiary (3^0) depending on the type of carbon atom to which they are bonded.

- A *primary hydrogen* is on a C bonded to one other C atom.
- A *secondary hydrogen* is on a C bonded to two other C atoms.
- A *tertiary hydrogen* is on a C bonded to three other C atoms.



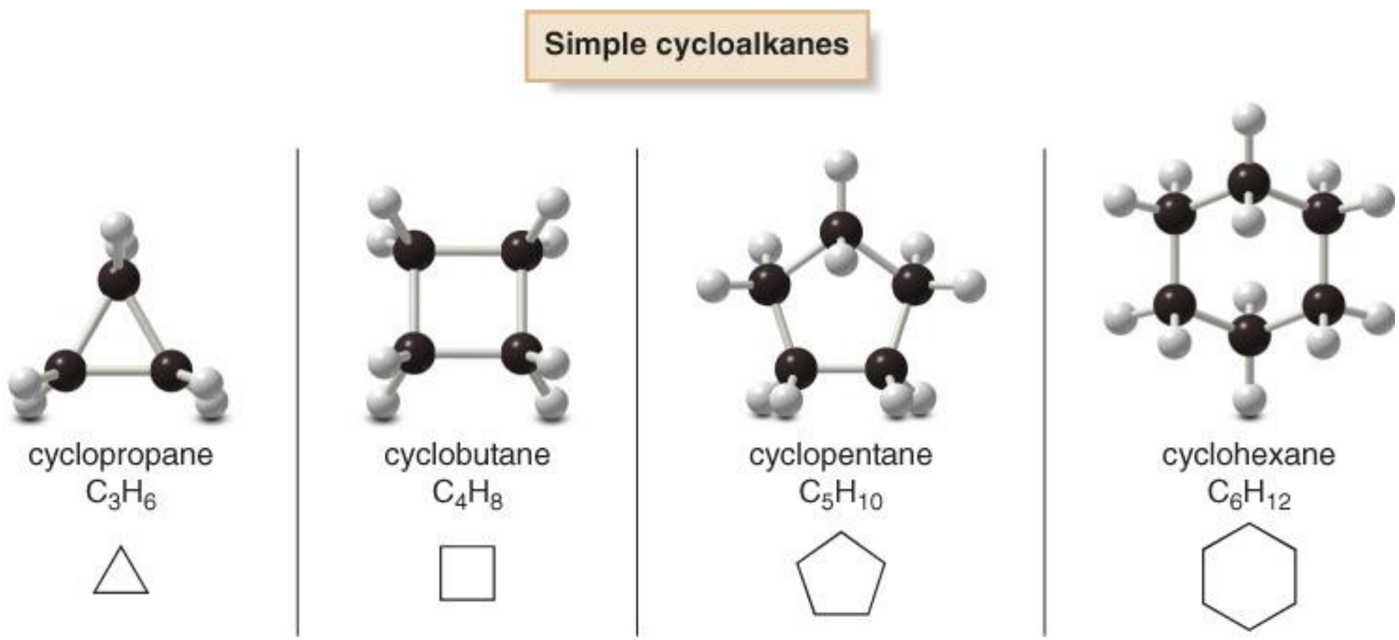
- The maximum number of possible constitutional isomers increases dramatically as the number of carbon atoms in the alkane increases.
  - 75 possible isomers for 10 carbons
  - 366,319 possible isomers for 20 carbons.
- The suffix “ane” identifies a molecule as an alkane.
- By increasing the number of carbons in an alkane by a CH_2 group (“methylene”) , one obtains a “homologous series” of alkanes.

TABLE 4.1 Summary: Straight-Chain Alkanes

Number of C atoms	Molecular formula	Name (*n*-alkane)	Number of constitutional isomers
1	CH_4	methane	—
2	C_2H_6	ethane	—
3	C_3H_8	propane	—
4	C_4H_{10}	butane	2
5	C_5H_{12}	pentane	3
6	C_6H_{14}	hexane	5
7	C_7H_{16}	heptane	9
8	C_8H_{18}	octane	18
9	C_9H_{20}	nonane	35
10	$C_{10}H_{22}$	decane	75
20	$C_{20}H_{42}$	eicosane	366,319

Cycloalkanes have molecular formula C_nH_{2n} and contain carbon atoms arranged in a ring.

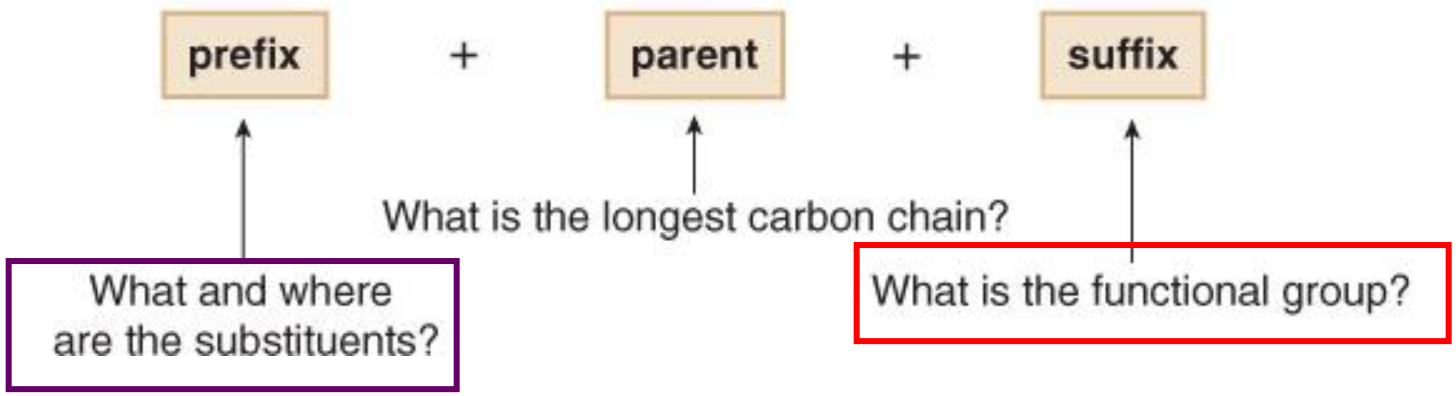
Simple cycloalkanes are named by adding the prefix *cyclo-* to the name of the acyclic alkane having the same number of carbons.



Nomenclature

The name of every organic molecule has 3 parts:

1. The parent name indicates the number of carbons in the longest continuous chain
2. The suffix indicates what functional group is present
3. The prefix tells us the identity, location, and number of substituents attached to the carbon chain

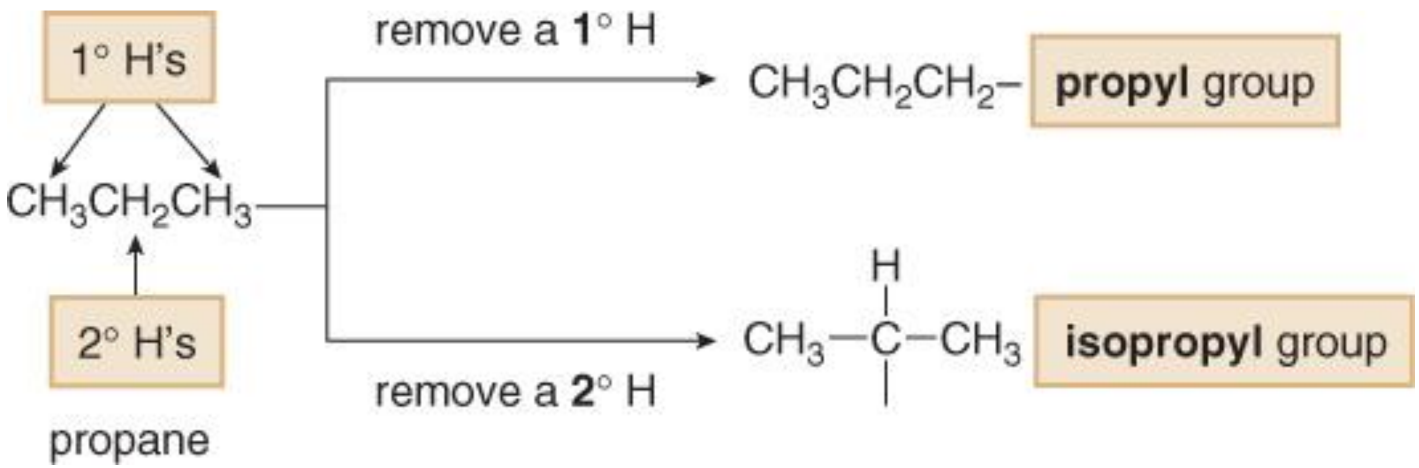


Nomenclature

- Carbon substituents bonded to a long carbon chain are called alkyl groups.
- An alkyl group is formed by removing one H atom from an alkane.
- To name an alkyl group, change the –*ane* ending of the parent alkane to –*yl*.
    - methane (CH_4) becomes methyl (CH_3-)
    - ethane (CH_3CH_3) becomes ethyl (CH_3CH_2-).

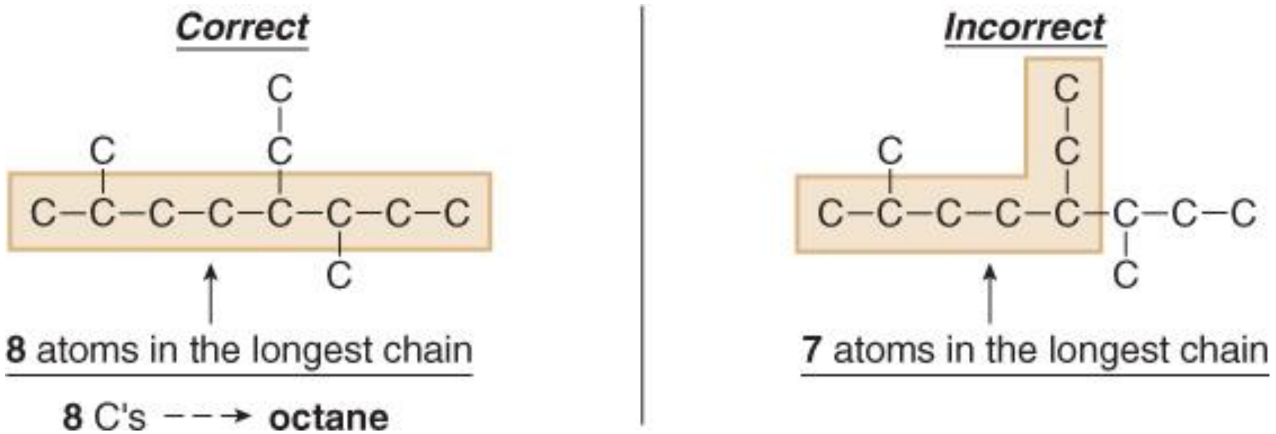
Naming three- or four-carbon alkyl groups is more complicated because the parent hydrocarbons have more than one type of hydrogen atom.

Propane has both 1^0 and 2^0 H atoms, and removal of each of these H atoms forms a different alkyl group with a different name.

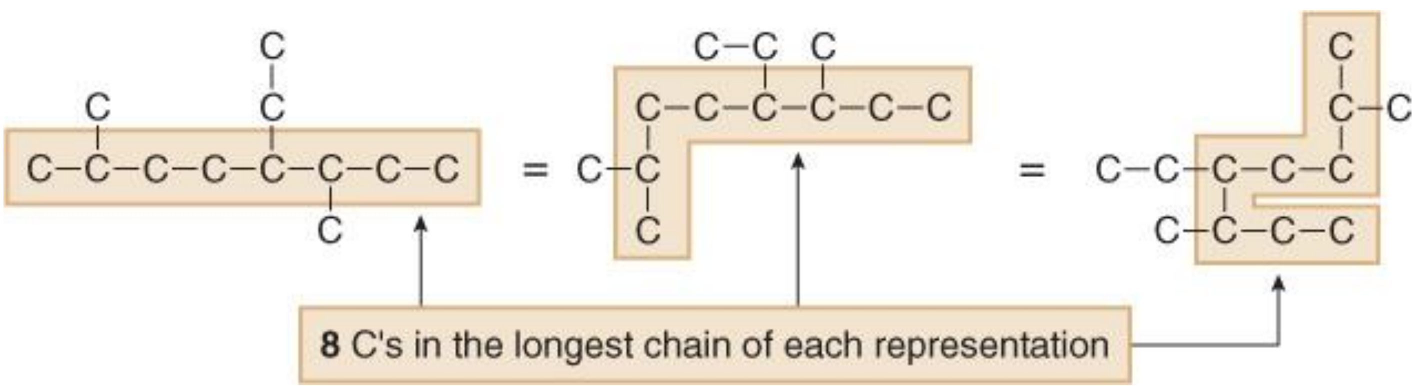


Rules for Naming Alkanes

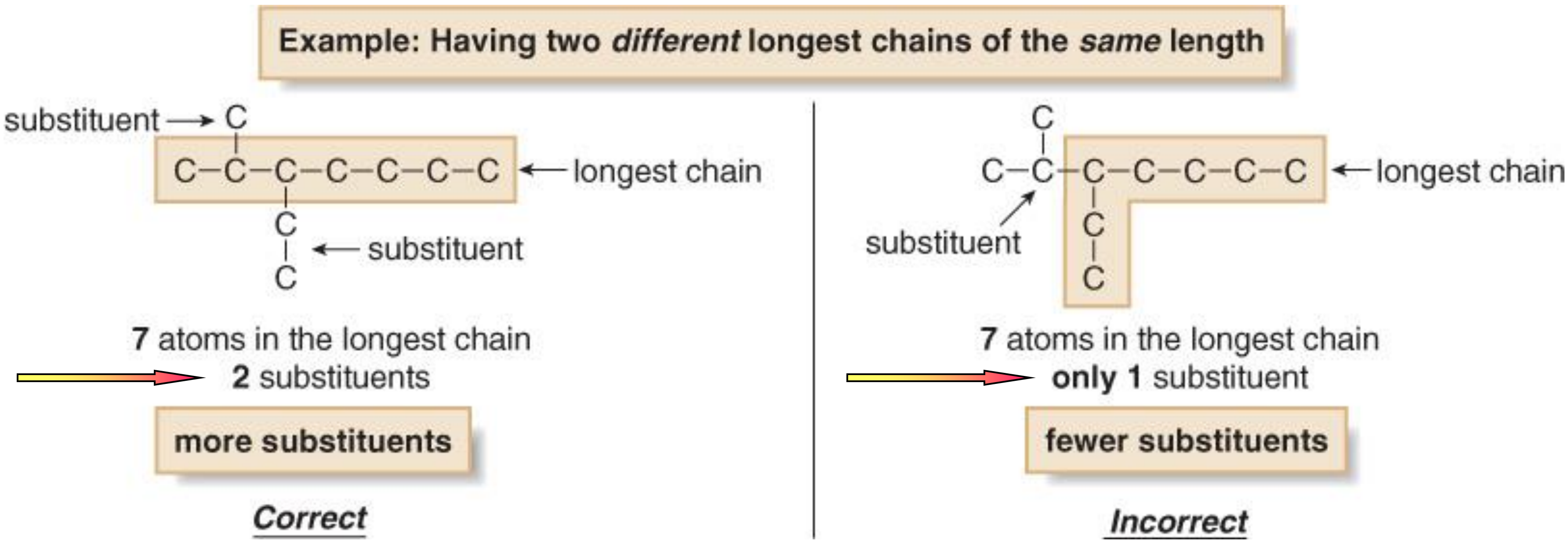
1. Find the parent carbon chain and add the suffix.



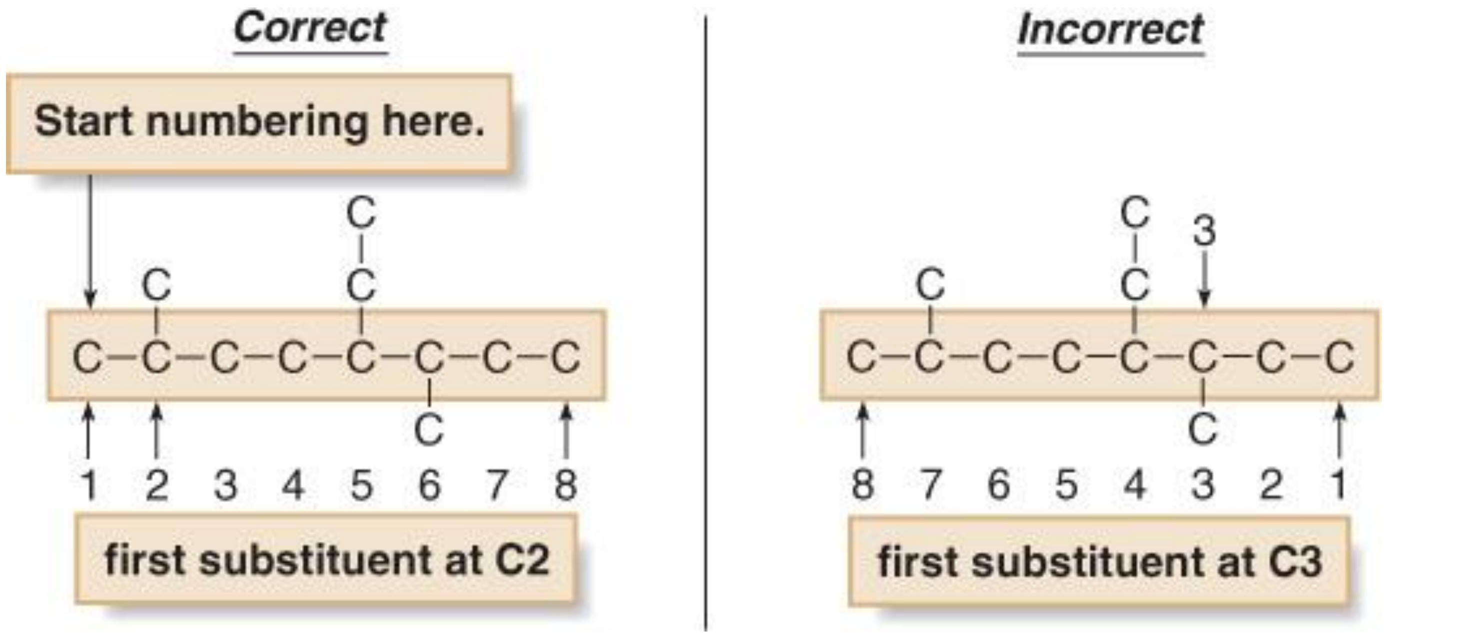
It does not matter if the chain is straight or it bends.



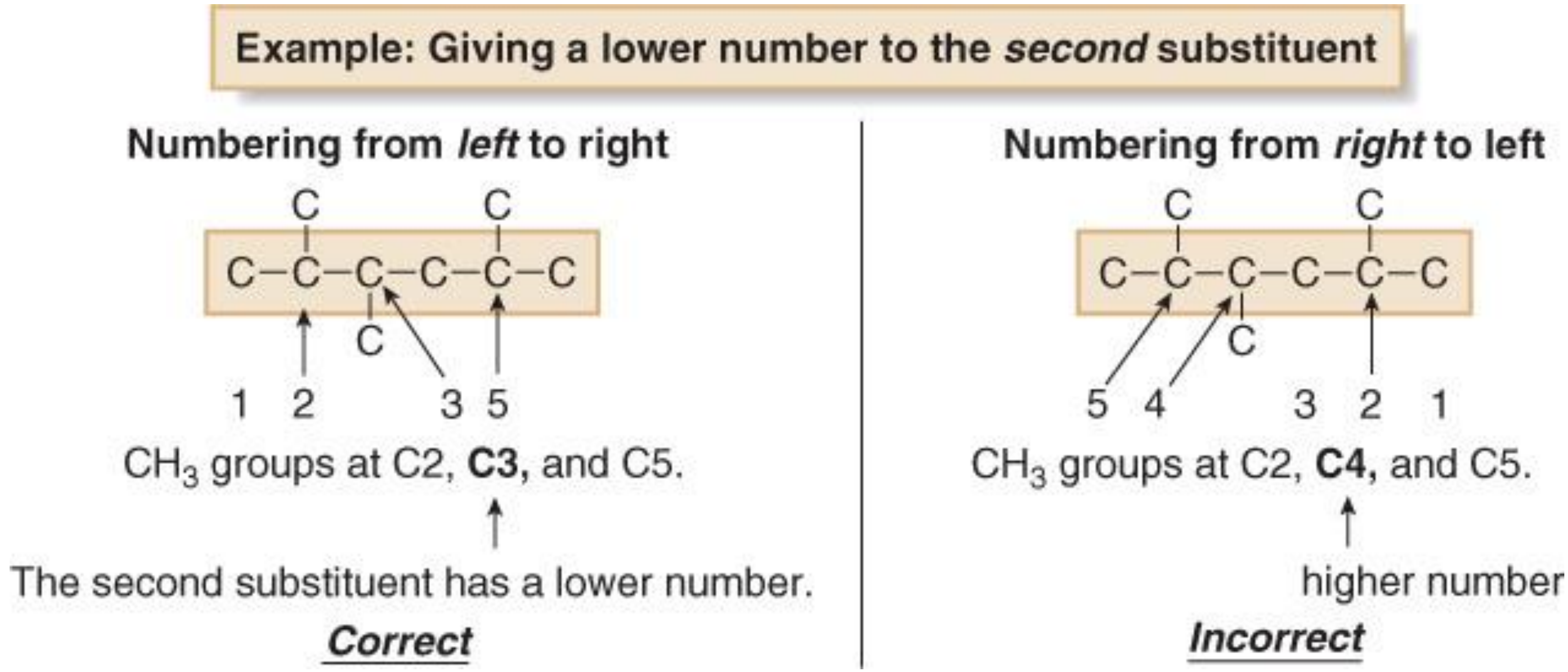
If there are two chains of equal length, pick the chain with greater number of substituents.



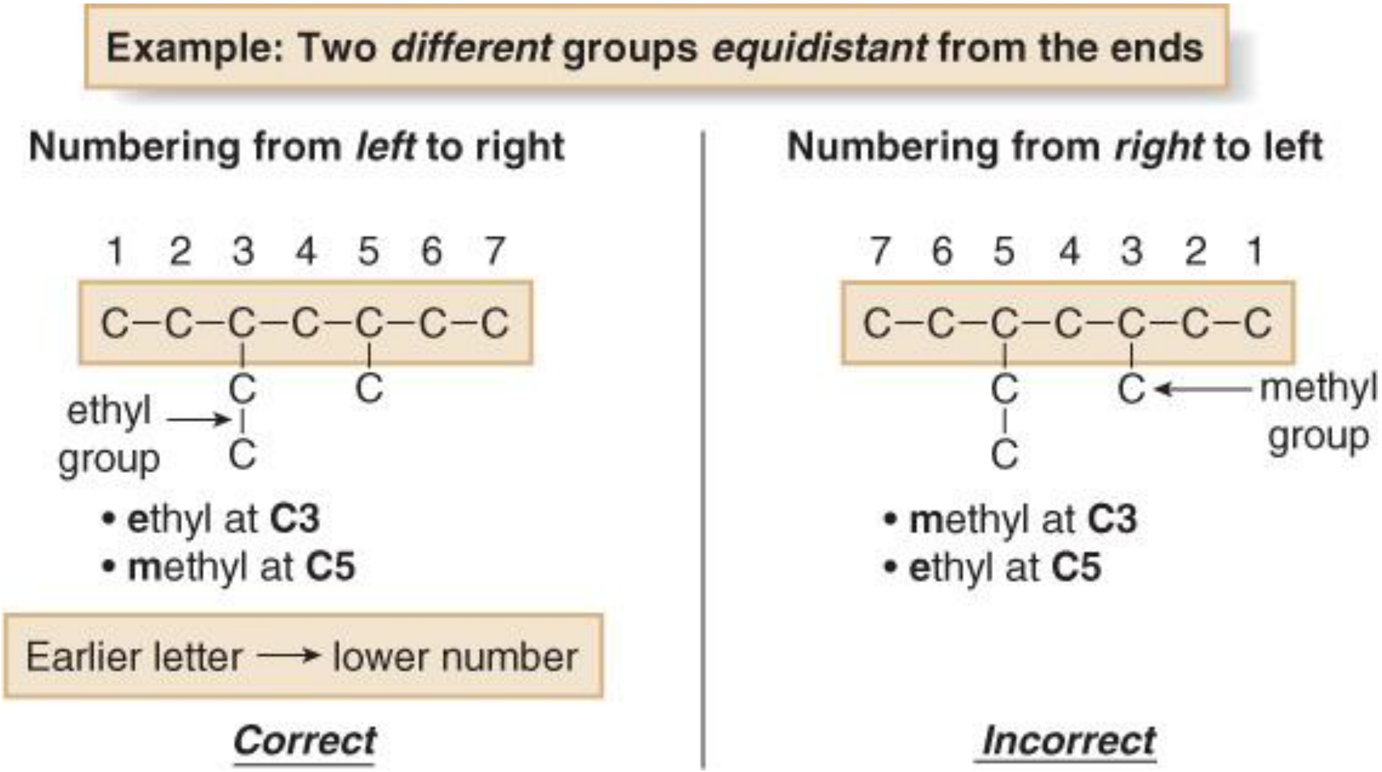
2. Number the atoms in the carbon chain to give the first substituent the lowest number.



If the first substituent is the same distance from both ends, number the chain to give the second substituent the lower number.

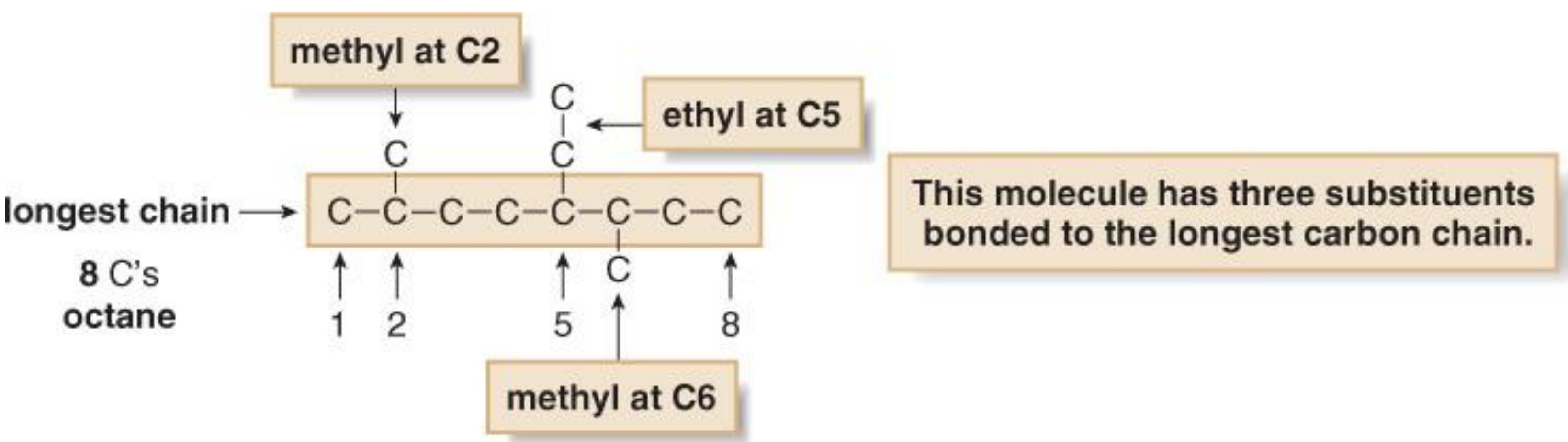


When numbering a carbon chain results in the same numbers from either end of the chain, assign the lower number alphabetically to the first substituent.



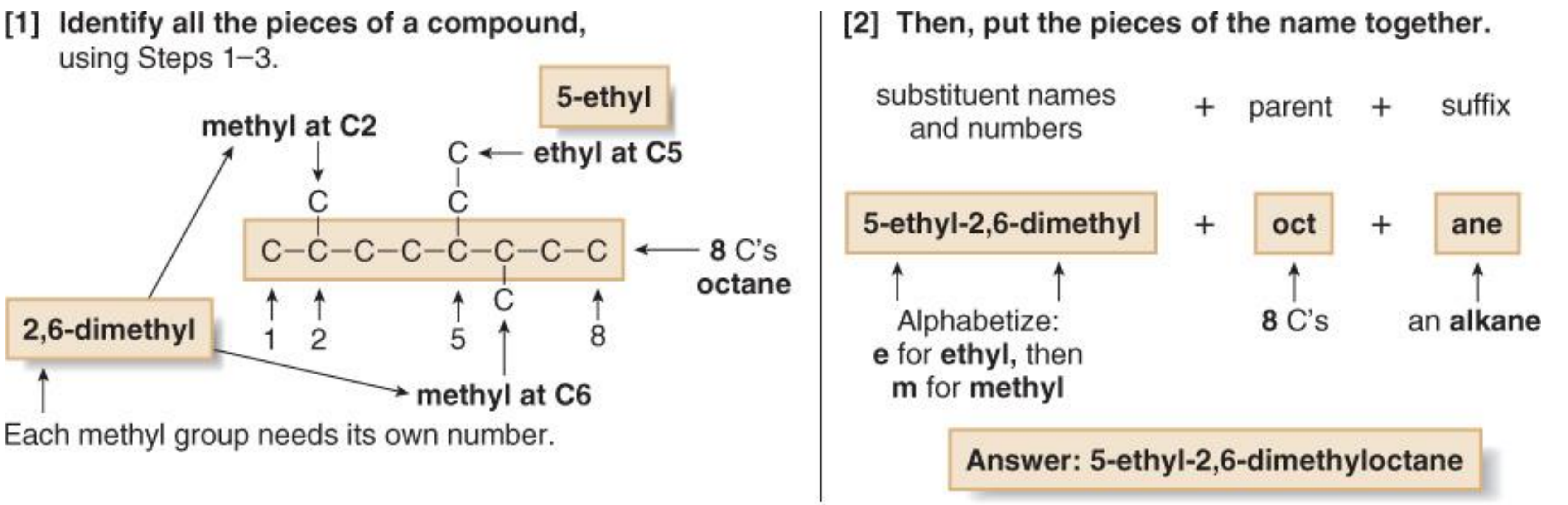
3. Name and number the substituents.

- Name the substituents as alkyl groups.
- Every carbon belongs to either the longest chain or a substituent, not both.
- Each substituent needs its own number
- If two or more identical substituents are bonded to the longest chain, use prefixes to indicate how many: di- for two groups, tri- for three groups, tetra- for four groups, and so forth.

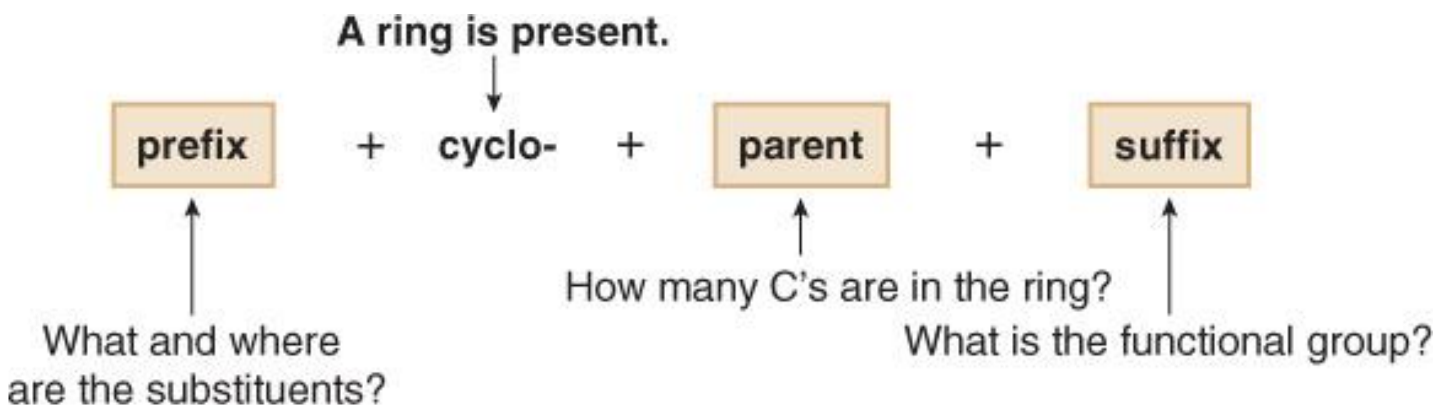


4. Combine substituent names and numbers + parent and suffix.

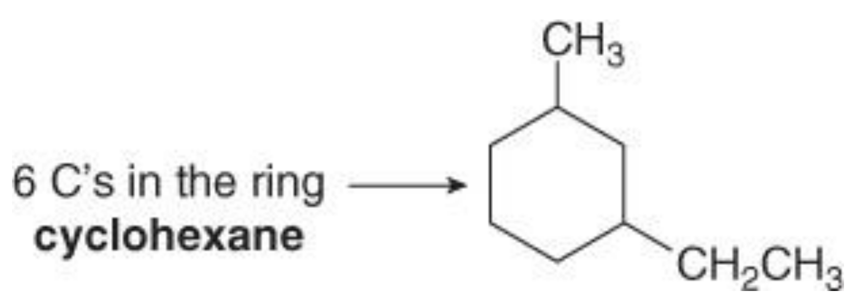
- Precede the name of the parent by the names of the substituents.
- Alphabetize the names of the substituents, ignoring all prefixes except iso, as in isopropyl and isobutyl.
- Precede the name of each substituent by the number that indicates its location.
- Separate numbers by commas and separate numbers from letters by hyphens. The name of an alkane is a single word, with no spaces after hyphens and commas.



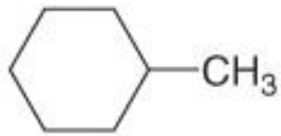
Cycloalkanes are named by using similar rules, but the prefix cyclo- immediately precedes the name of the parent.



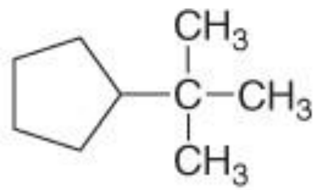
1. Find the parent cycloalkane.



2. Name and number the substituents. No number is needed to indicate the location of a single substituent.



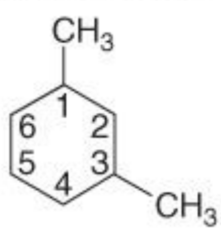
methylcyclohexane



tert-butylcyclopentane

For rings with more than one substituent, begin numbering at one substituent and proceed around the ring to give the second substituent the lowest number.

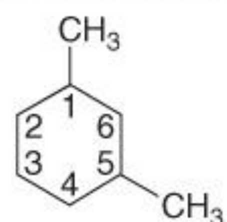
numbering clockwise



CH_3 groups at C1 and **C3**
The 2nd substituent has a lower number.

Correct: **1,3-dimethylcyclohexane**

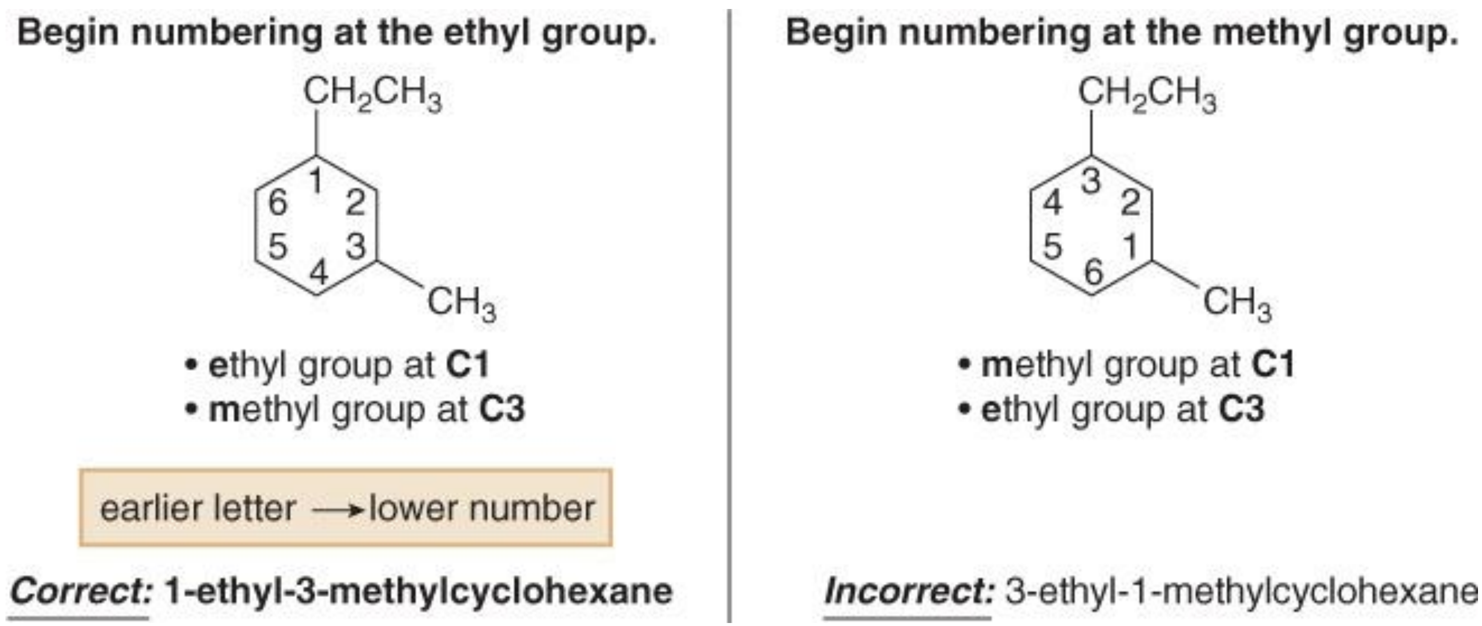
numbering counterclockwise



CH_3 groups at C1 and **C5**

Incorrect: 1,5-dimethylcyclohexane

With two different substituents, number the ring to assign the lower number to the substituents alphabetically.

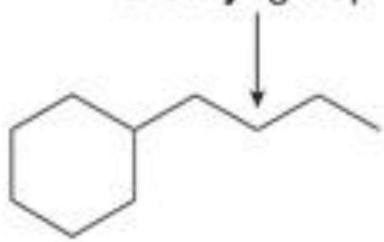


In the case of an alkane composed of both a ring and a long chain. If the number of carbons in the ring is greater than or equal to the number of carbons in the longest chain, the compound is named as a cycloalkane.

Contrast two different examples

more carbons in the ring

4 C's in the chain — a **butyl** group



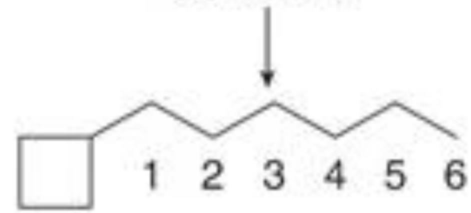
6 C's in the ring—**cyclohexane**

Name as a **cyclohexane** with a substituent.

Answer: butylcyclohexane

more carbons in the chain

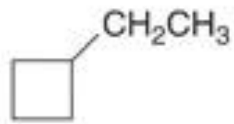
6 C's in the chain — a **hexane**



4 C's in the ring—a **cyclobutyl** group

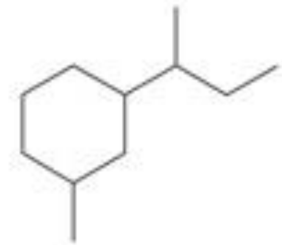
Name as a *hexane* with a substituent.

Answer: 1-cyclobutylhexane



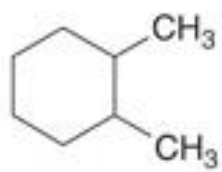
ethylcyclobutane

[No number is needed with only one substituent.]



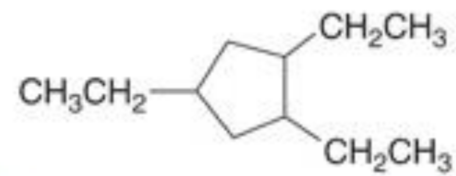
1-*sec*-butyl-3-methylcyclohexane

[Assign the lower number to the 1st substituent alphabetically: the **b** of **b**utyl before the **m** of **m**ethyl.]



1,2-dimethylcyclohexane

[Number to give the 2nd CH_3 group the lower number: 1,2- not 1,6-.]



1,2,4-triethylcyclopentane

[Number to give the 2nd CH_3CH_2 group the lower number: 1,2,4- not 1,3,4- or 1,3,5-.]

Physical Properties of Alkanes

TABLE 4.2 Physical Properties of Alkanes

Property	Observation
Boiling point	• Alkanes have low bp's compared to more polar compounds of comparable size. **low bp** → $CH_3CH_2CH_3$: VDW, MW = 44, bp = –42 °C; CH_3CHO: VDW, DD, MW = 44, bp = 21 °C; CH_3CH_2OH: VDW, DD, HB, MW = 46, bp = 79 °C **Increasing strength of intermolecular forces** **Increasing boiling point**
	• Bp increases as the number of carbons increases because of increased surface area. $CH_3CH_2CH_2CH_3$: bp = 0 °C; $CH_3CH_2CH_2CH_2CH_3$: bp = 36 °C; $CH_3CH_2CH_2CH_2CH_2CH_3$: bp = 69 °C **Increasing surface area** **Increasing boiling point**

Physical Properties of Alkanes:

TABLE 4.2 Continued

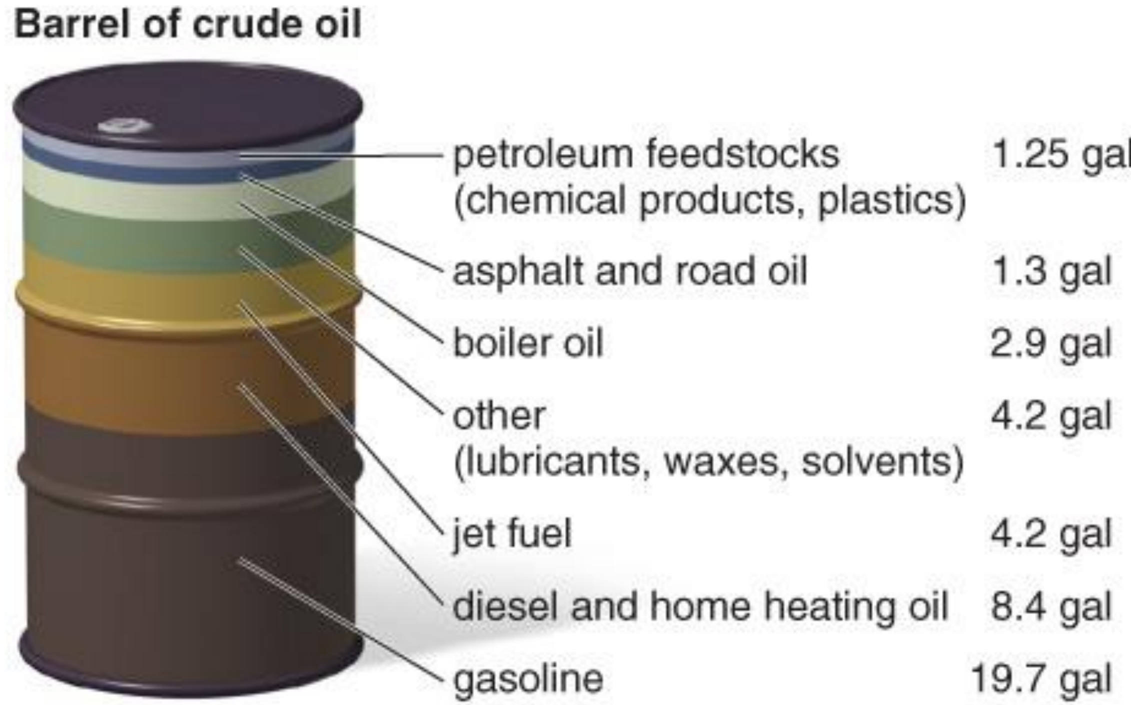
	• The bp of isomers decreases with branching because of decreased surface area. ← **Increasing branching** $CH_3-C(CH_3)_2-CH_3$ bp = 10 °C; $CH_3CH(CH_3)CH_2CH_3$ bp = 30 °C; $CH_3CH_2CH_2CH_2CH_3$ bp = 36 °C → **Increasing surface area** **Increasing boiling point**
Melting point	• Alkanes have low mp's compared to more polar compounds of comparable size. $CH_3CH_2CH_3$, VDW, MW = 44, mp = −190 °C (low mp); CH_3CHO, VDW, DD, MW = 44, mp = −121 °C → **Increasing strength of intermolecular forces** **Increasing melting point**
	• Mp increases as the number of carbons increases because of increased surface area. $CH_3CH_2CH_2CH_3$ mp = −138 °C; $CH_3CH_2CH_2CH_2CH_2CH_3$ mp = −95 °C → **Increasing surface area** **Increasing melting point**
	• Mp increases with increased symmetry. $CH_3CH_2CH(CH_3)_2$ mp = −160 °C; $(CH_3)_4C$ mp = −17 °C → **Increasing symmetry** **Increasing melting point**
Solubility	• Alkanes are soluble in organic solvents. • Alkanes are insoluble in water.

Key: **bp** = boiling point; **mp** = melting point; **VDW** = van der Waals; **DD** = dipole–dipole; **HB** = hydrogen bonding; **MW** = molecular weight

Fossil Fuels:

Many alkanes occur in nature, primarily in natural gas and petroleum.

Natural gas is com-posed largely of methane, with lesser amounts of ethane, propane and butane.



Petroleum is a complex mixture of compounds, most of which are hydrocarbons containing one to forty carbon atoms. Distilling crude petroleum (called refining), separates it into usable fractions that differ in boiling point.

gasoline: C_5H_{12}—$C_{12}H_{26}$

kerosene: $C_{12}H_{26}$—$C_{16}H_{34}$

diesel fuel: $C_{15}H_{32}$—$C_{18}H_{38}$

Fossil Fuels:

Figure 4.5 Refining crude petroleum into usable fuel and other petroleum products. (a) An oil refinery. At an oil refinery, crude petroleum is separated into fractions of similar boiling point by the process of distillation. (b) Schematic of a refinery tower. As crude petroleum is heated, the lower-boiling, more volatile components distill first, followed by fractions of progressively higher boiling point.