2. Alkanes: The Nature of Organic Compounds

스마트헬스케어학부 의공학전공

임해균 교수

2. Alkanes: The Nature of Organic Compounds

2.3 Naming Branched-Chain Alkanes

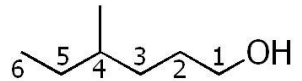
- Compounds are given systematic names by a process that uses IUPAC rule

Prefix — Parent — Locant — Suffix

Prefix	Parent	Locant	Suffix
Where and what are the substituents?	How many carbons?	Where is the primary functional group?	What is the primary functional group?

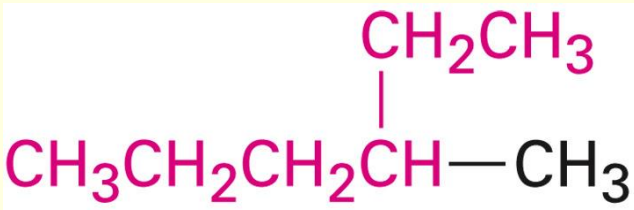
1. Find parent hydrocarbon chain
2. Number the atoms in the main chain
3. Identify and number the substituents
4. Write the name as a single word

- IUPAC substitutive nomenclature: a name may have as many as four features
  - Locants, prefixes, parent compound, and suffixes



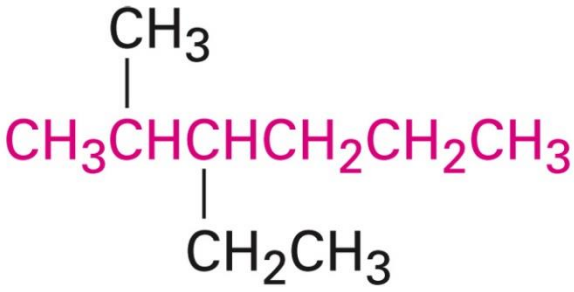
4-Methyl-1-hexanol

1. Find parent hydrocarbon chain



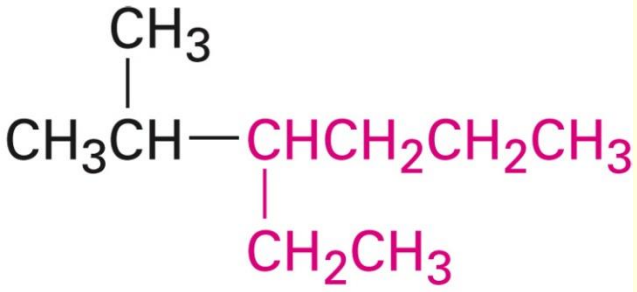
Named as a substituted hexane

Find the **longest continuous carbon** chain in the molecule and use the name of that chain as the parent name. The longest chain may not always be obvious; you may have to "turn corners."



Named as a hexane with *two* substituents

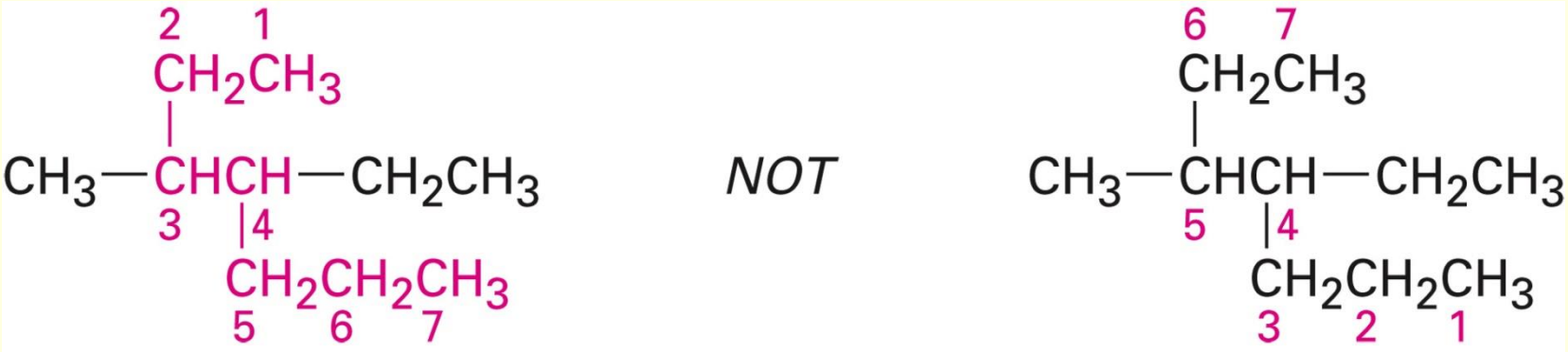
NOT



as a hexane with *one* substituent

If two chains of equal length are present, choose the one with the **larger number of branch points** as the parent.

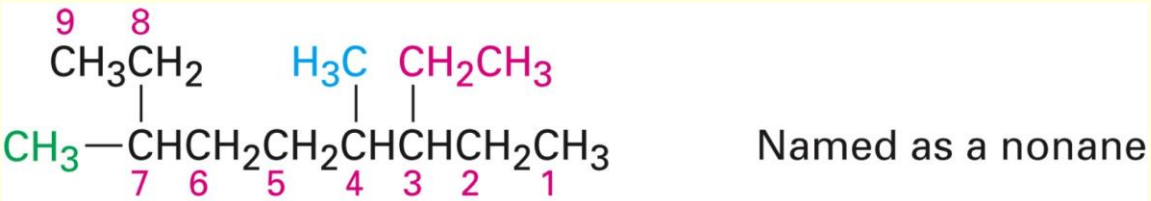
2. Number the atoms in the main chain



Beginning at the end **nearer the first branch** point, number each carbon atom in the parent chain.

The first branch occurs at C3 in the proper system of numbering but at C4 in the improper system.

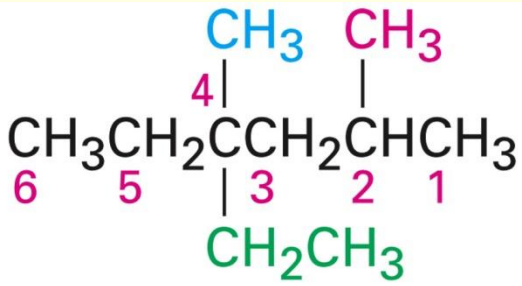
3. Identify and number the substituents



Named as a nonane

Substituents: On C3, CH_2CH_3 (3-ethyl)
On C4, CH_3 (4-methyl)
On C7, CH_3 (7-methyl)

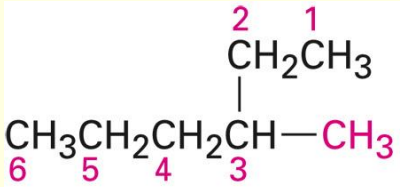
Assign a number, called a *locant,* to each substituent to specify its point of attachment to the parent chain. If there are two substituents on the same carbon, assign them both the same number. There must always be as many numbers in the name as there are substituents.



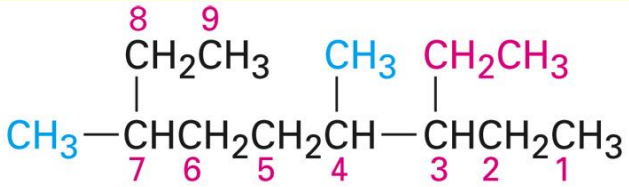
Named as a hexane

Substituents: On C2, CH_3 (2-methyl)
On C4, CH_3 (4-methyl)
On C4, CH_2CH_3 (4-ethyl)

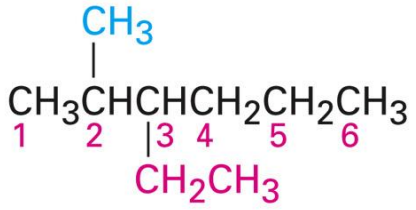
4. Write the name as a single word



3-Methylhexane

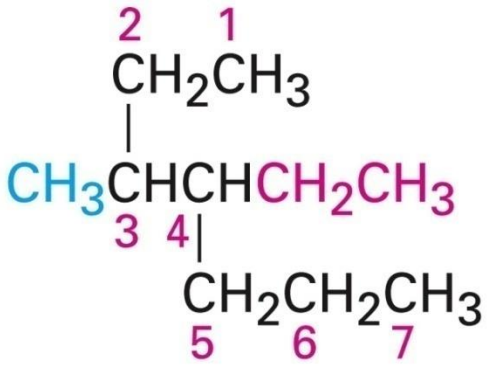


3-Ethyl-4,7-dimethylnonane

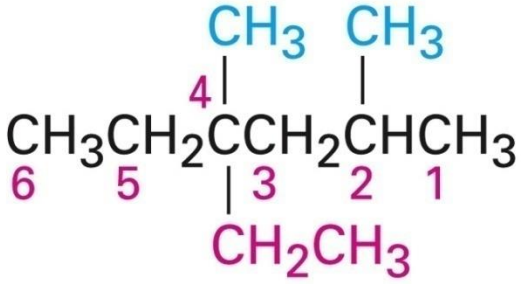


3-Ethyl-2-methylhexane

Use hyphens to separate the various prefixes and commas to separate numbers. If two or more different side chains are present, cite them in **alphabetical order.** If two or more identical side chains are present, use the appropriate **multiplier prefi xes *di-*, *tri-*, *tetra-*, and so forth.**
Don't use these prefixes for alphabetizing, though.

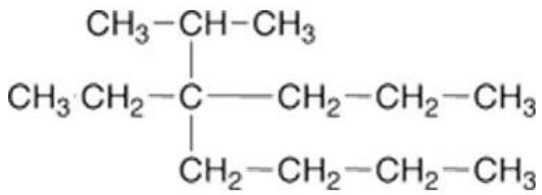


4-Ethyl-3-methylheptane



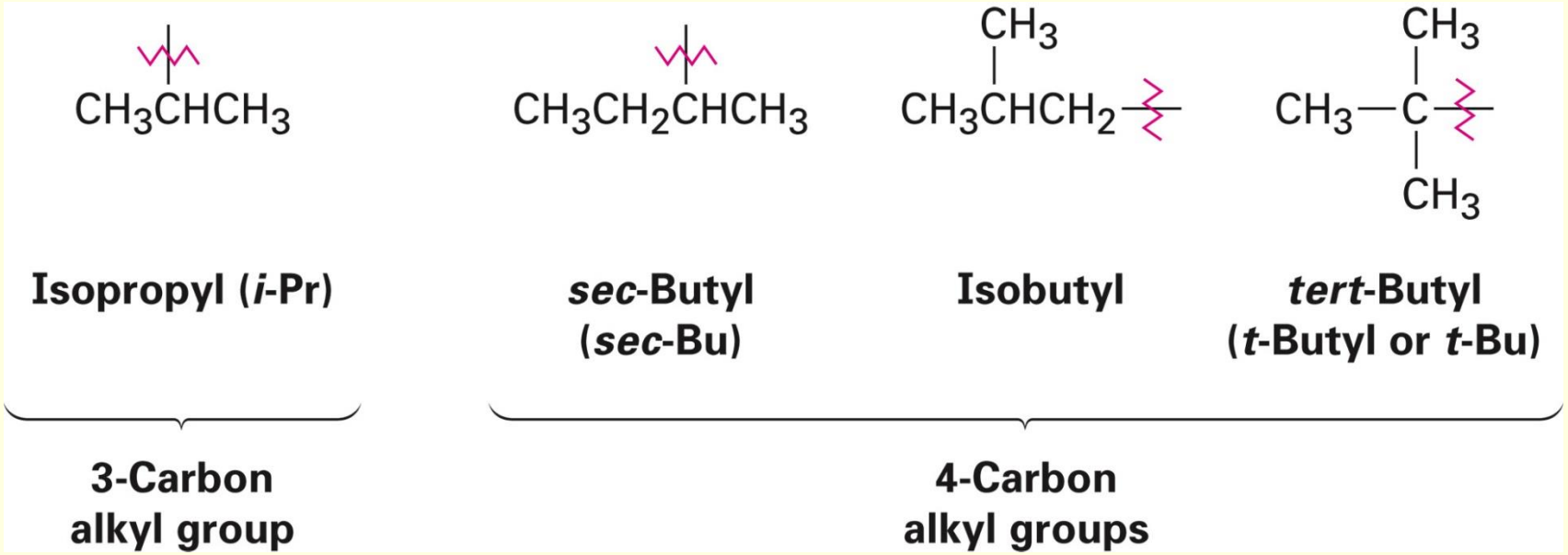
4-Ethyl-2,4-dimethylhexane

- *Di-*, *tri-*, *tetra-*, and hyphenated prefixes *tert-* and *sec-* are ignored
- *Iso-, neo-, cyclo-* are **not** ignored



23

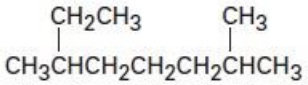
Common names



Worked Example 2.2

Naming an Alkane

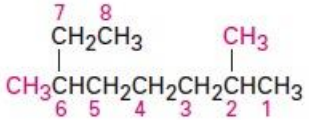
What is the IUPAC name of the following alkane?



Strategy

The molecule has a chain of eight carbons (octane) with two methyl substituents. Numbering from the end nearer the first methyl substituent indicates that the methyls are at C2 and C6.

Solution



2,6-Dimethyloctane

Worked Example 2.3

Drawing a Structure from a Name

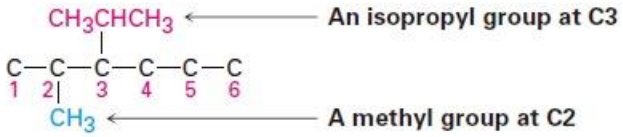
Draw the structure of 3-isopropyl-2-methylhexane.

Strategy

First, look at the parent name (hexane) and draw its carbon structure.

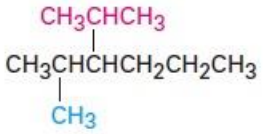
C–C–C–C–C–C **Hexane**

Next, find the substituents (3-isopropyl and 2-methyl), and place them on the proper carbons.



Finally, add hydrogens to complete the structure.

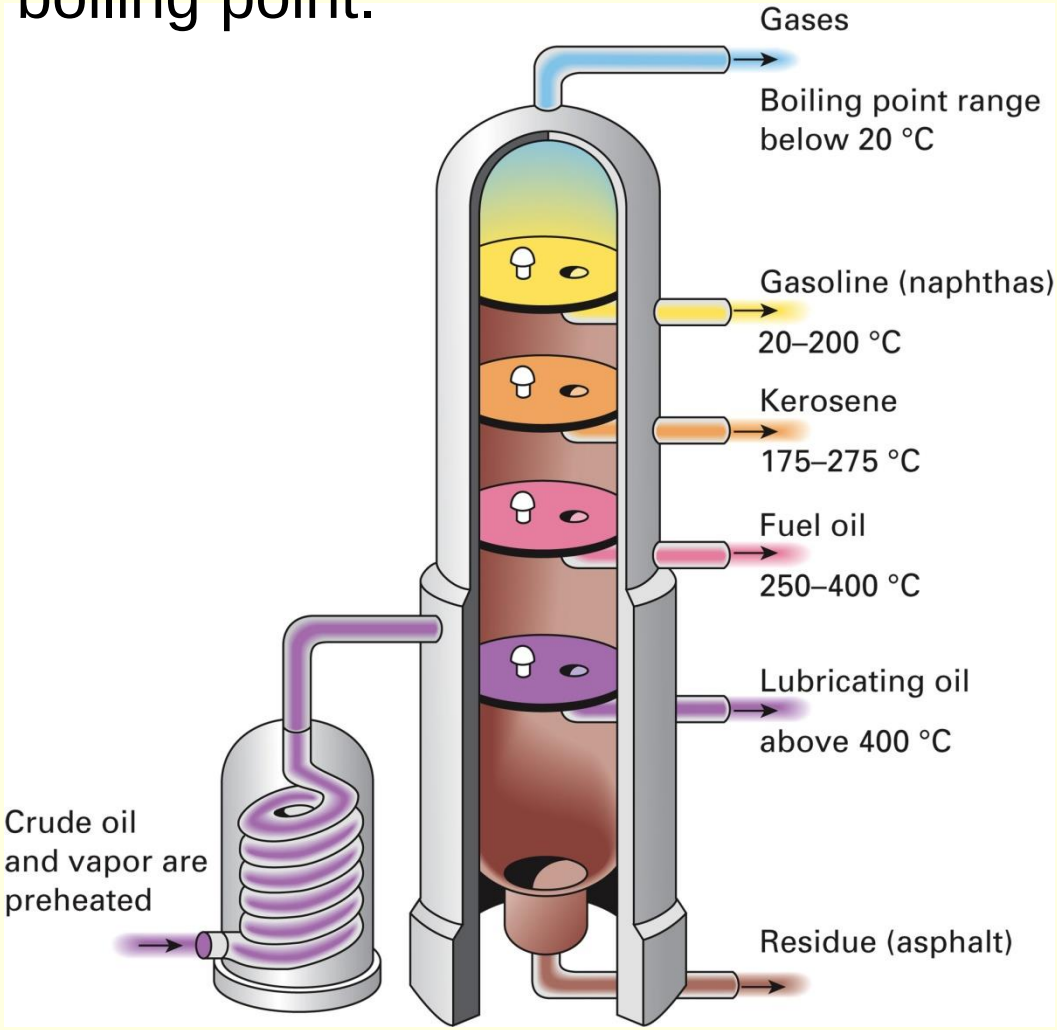
Solution



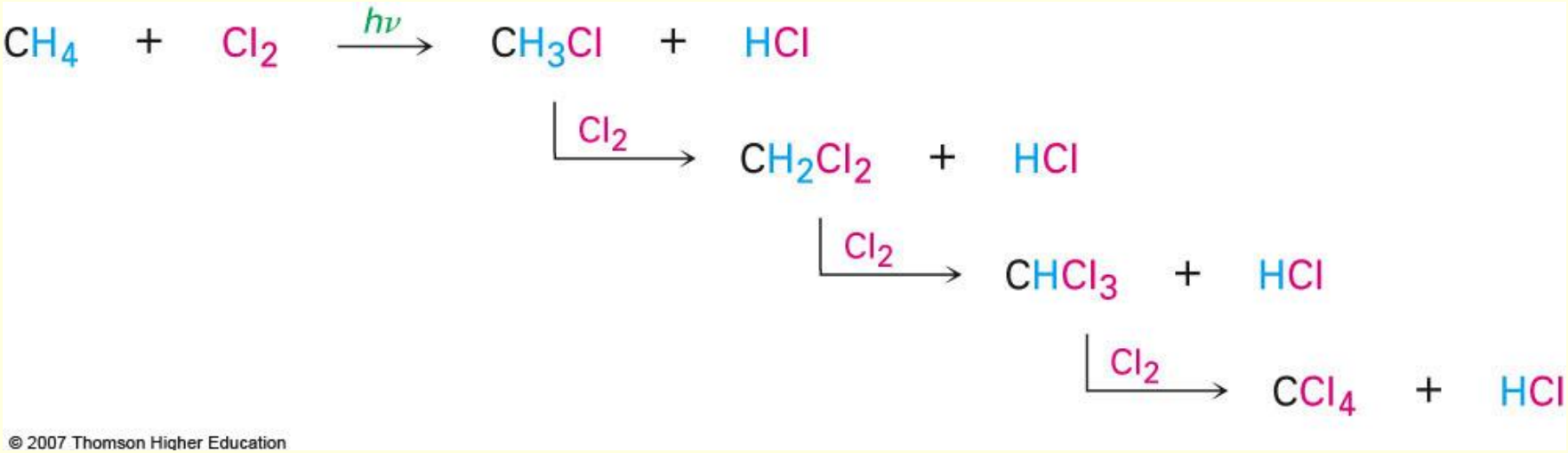
3-Isopropyl-2-methylhexane

2.4 Properties of Alkanes

Fractional distillation separates petroleum into fractions according to boiling point.

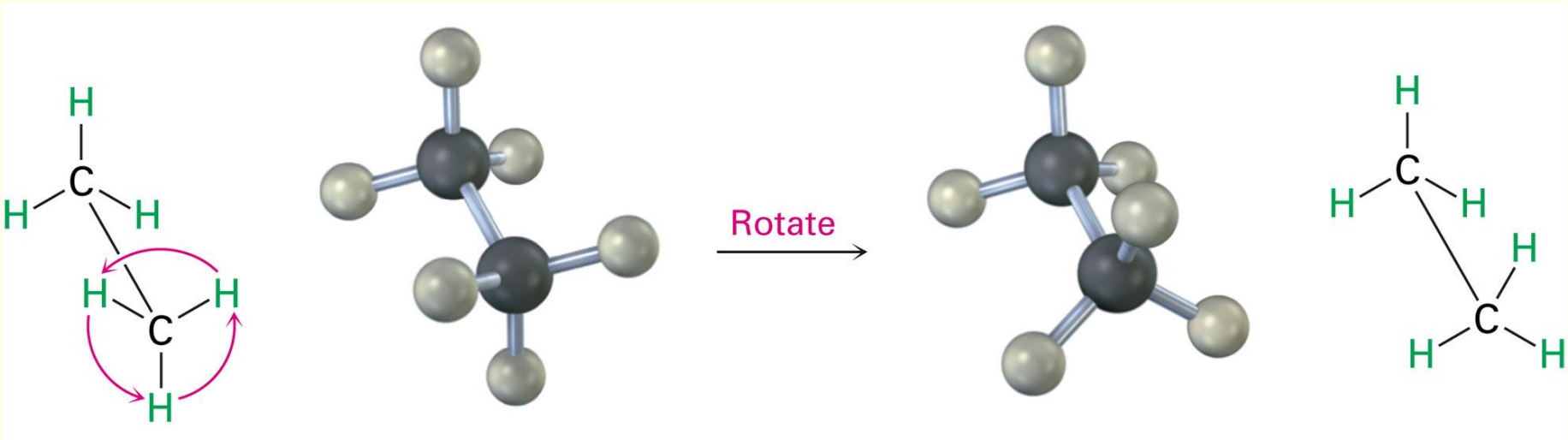


- Alkanes are sometimes called **paraffins** (low affinity compounds) because they do not react as most chemicals
- They will burn in a flame, producing carbon dioxide, water, and heat
- They react with Cl_2 in the presence of light to replace H's with Cl's (not controlled)

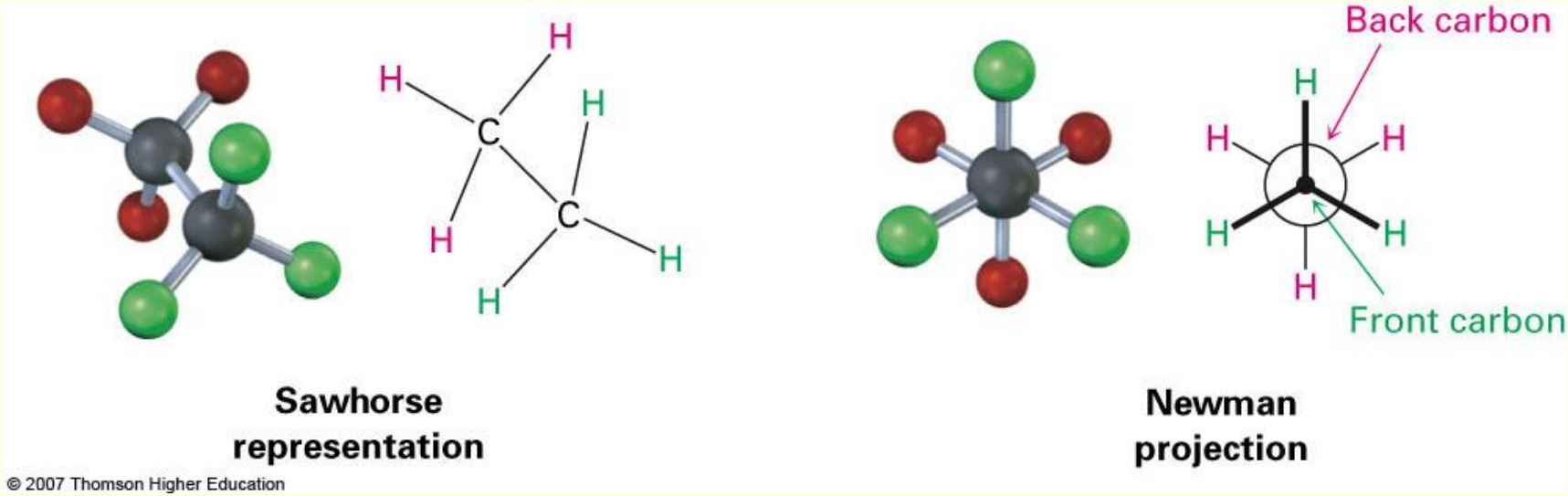


2.5 Conformations of Ethane

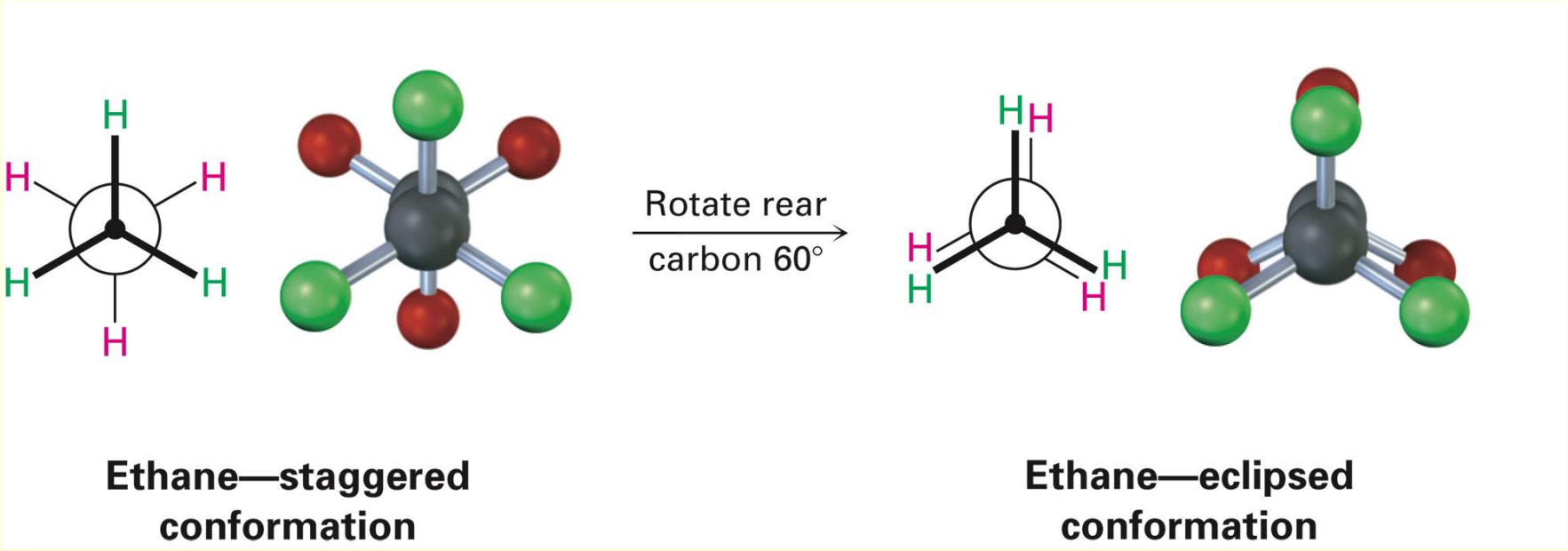
- Stereochemistry concerned with the 3-D aspects of molecules
- σ bonds are cylindrically symmetrical
- Rotation is possible around C-C bonds in open-chain molecules



- **Conformation**- Different arrangement of atoms resulting from bond rotation
- Conformations can be represented in 2 ways:



- There is a barrier to rotation, and some conformers are more stable than others
- **Staggered**- most stable: all 6 C-H bonds are as far away as possible
- **Eclipsed**- least stable: all 6 C-H bonds are as close as possible to each other



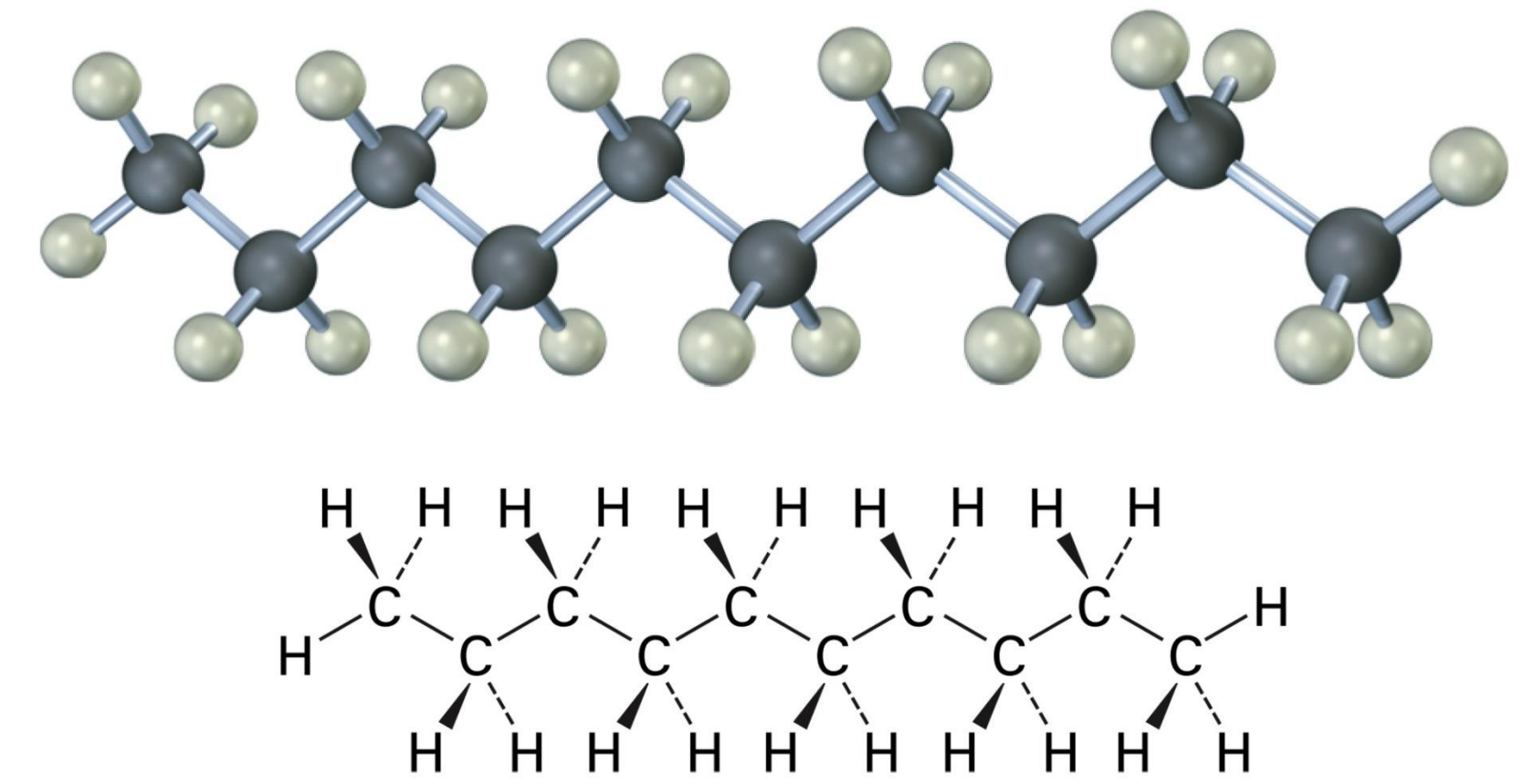


Figure 2.8 The **most stable conformation** of any alkane is the one in which the bonds on adjacent carbons are **staggered** and the carbon chain is **fully extended** so that large groups are far away from one another, as in this model of **decane**.

Worked Example 2.4

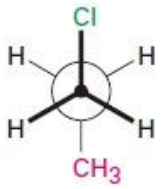
Drawing a Newman Projection

Sight along the C1–C2 bond of 1-chloropropane and draw Newman projections of the most stable and least stable conformations.

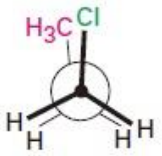
Strategy

The most stable conformation of a substituted alkane is generally a staggered one in which large groups are as far away from one another as possible. The least stable conformation is generally an eclipsed one in which large groups are as close as possible.

Solution



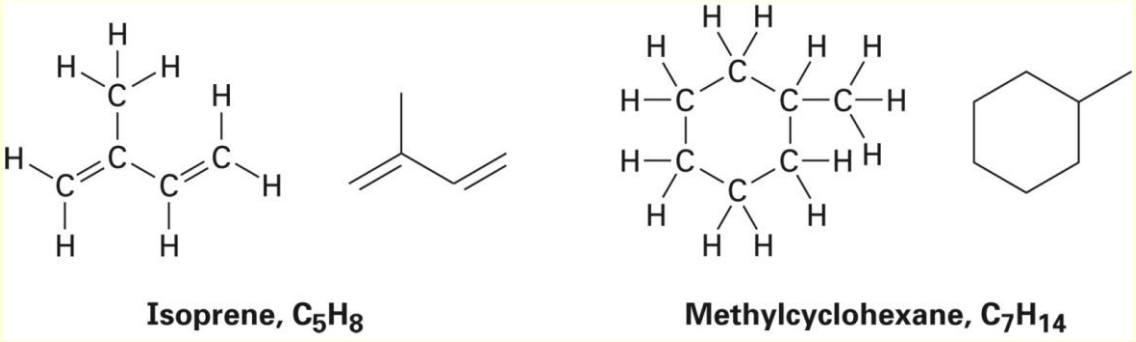
Most stable (staggered)

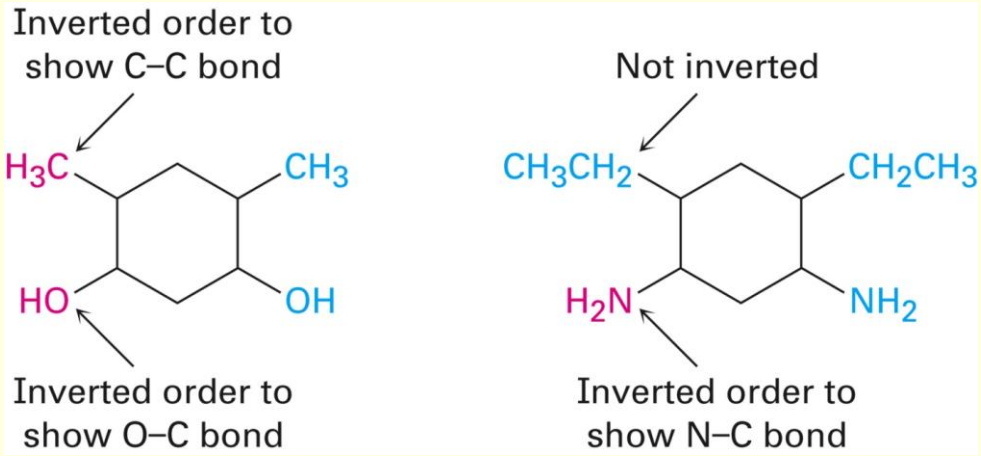


Least stable (eclipsed)

2.6 Drawing Chemical Structures

Skeletal structure



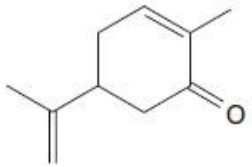


One further comment: although such groupings as CH_3, OH, and NH_2 are usually written with the C, O, or N atom first and the H atom second, the order of writing is sometimes inverted to H_3C, HO, and H_2N if needed to make the bonding connections in a molecule clearer. Larger units such as CH_2CH_3 are not inverted, though; we don't write H_3CH_2C because it would be confusing. There are, however, no well-defined rules that cover all cases; it's largely a matter of preference.

Worked Example 2.5

Interpreting a Skeletal Structure

Carvone, a substance responsible for the odor of spearmint, has the following structure. Tell how many hydrogens are bonded to each carbon, and give the molecular formula of carvone.

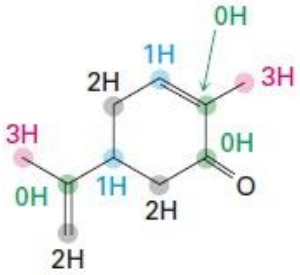


Carvone

Strategy

Remember that the end of a line represents a carbon atom with three hydrogens, CH_3; a two-way intersection is a carbon atom with two hydrogens, CH_2; a three-way intersection is a carbon atom with one hydrogen, CH; and a four-way intersection is a carbon atom with no attached hydrogens.

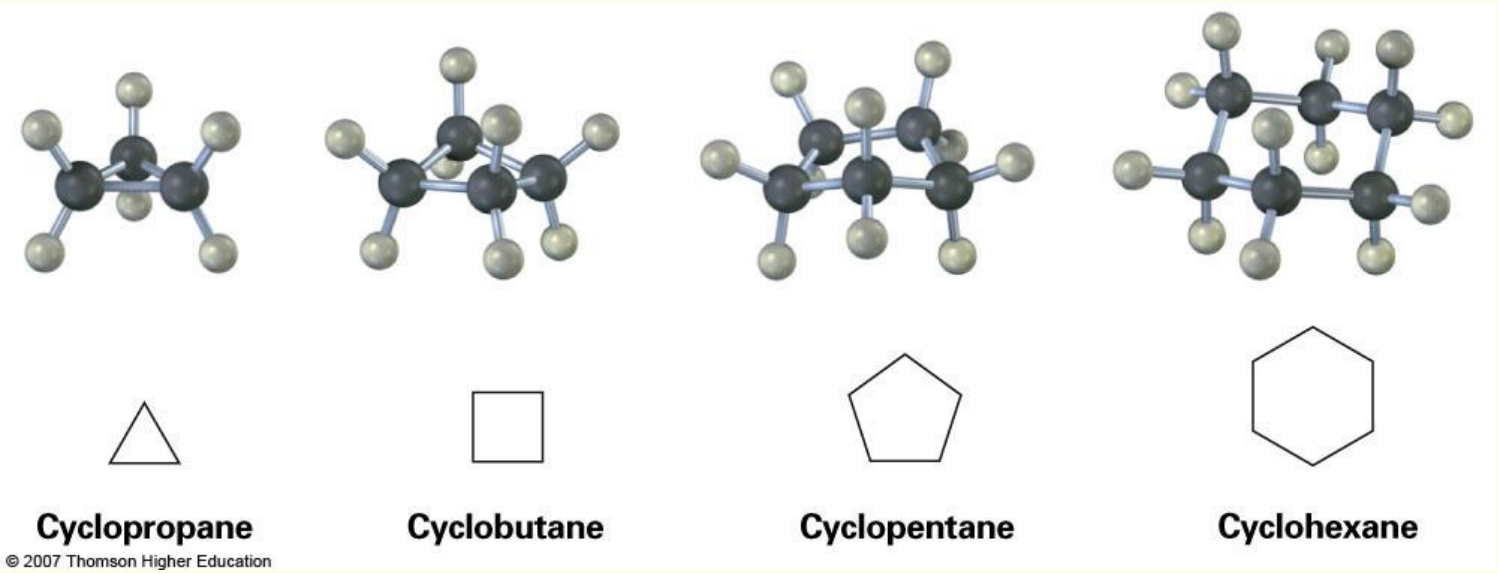
Solution



Carvone, $C_{10}H_{14}O$

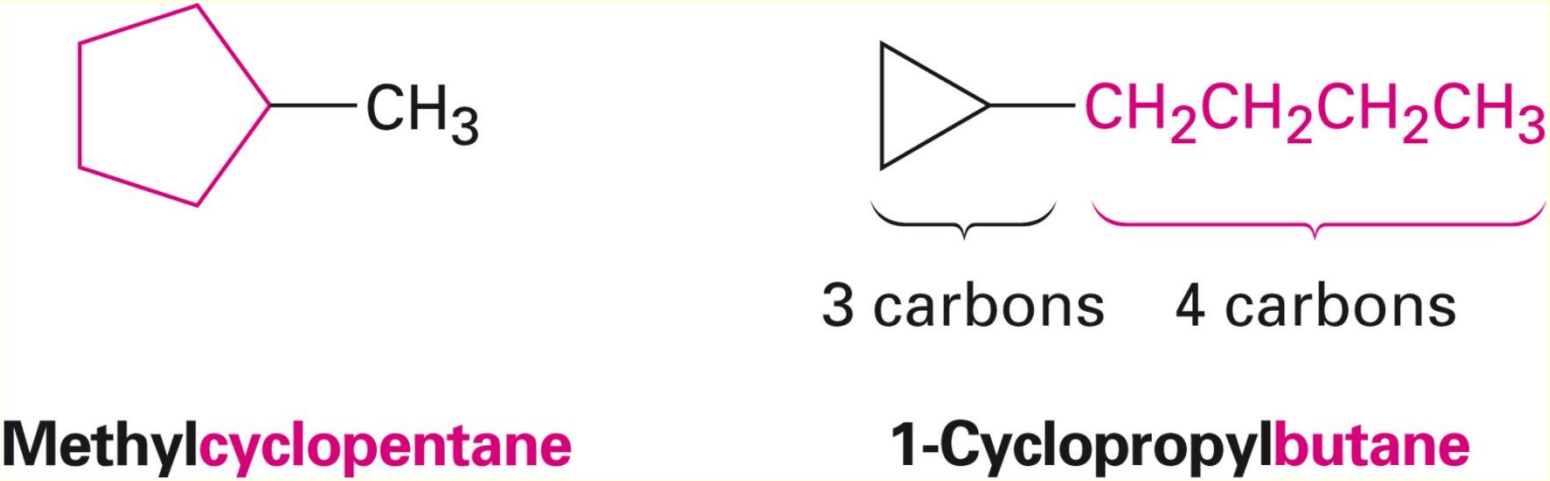
2.7 Cycloalkanes

- **Cycloalkanes** are saturated cyclic hydrocarbons
- Have the general formula (C_nH_{2n})



Naming Cycloalkanes

1. Find the parent. # of carbons in the ring.

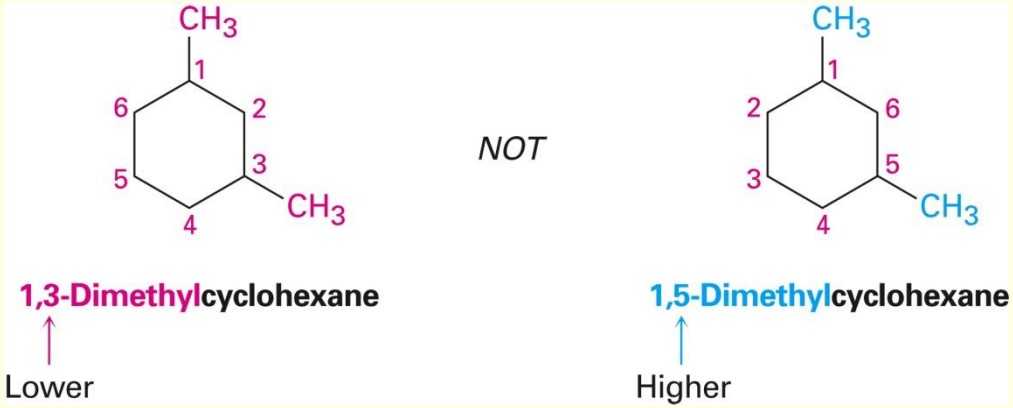


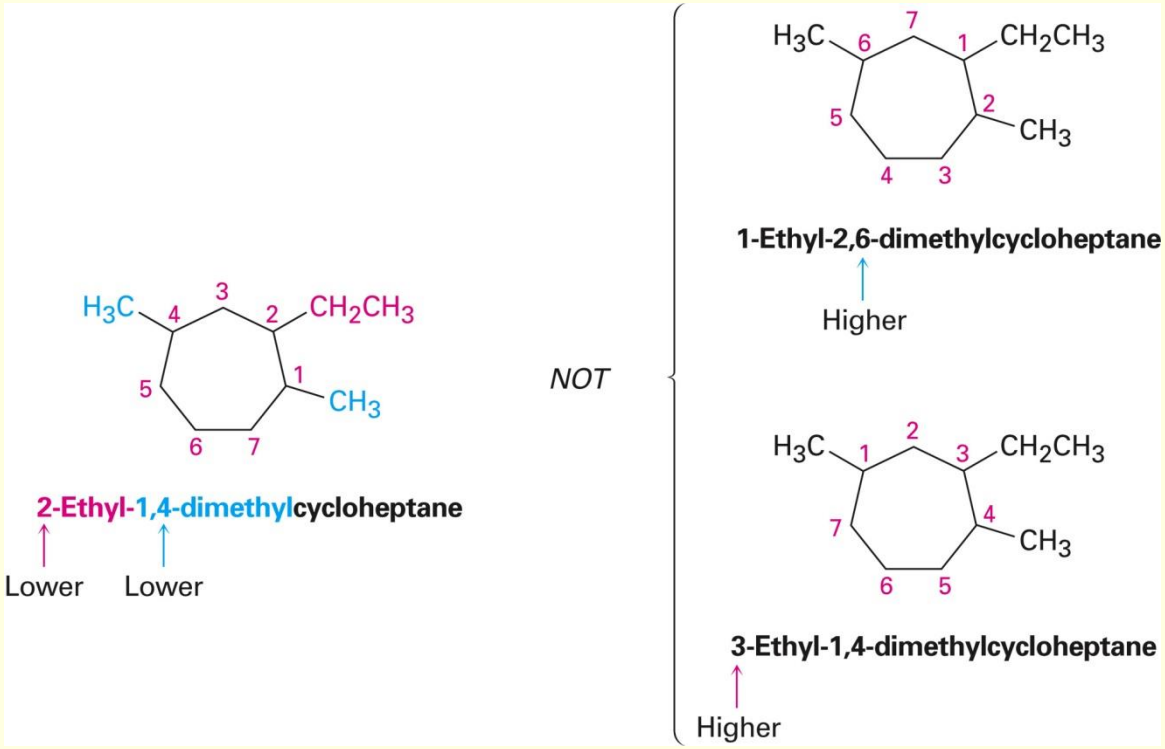
Count the number of carbon atoms in the **ring** and the number in the **largest substituent chain**.

If the number of carbon atoms in the ring is equal to or greater than the number in the substituent, the compound is named as an **alkyl-substituted cycloalkane.**

If the number of carbon atoms in the largest substituent is greater than the number in the ring, the compound is named as a **cycloalkyl-substituted alkane.**

2. Number the substituents, and write the name



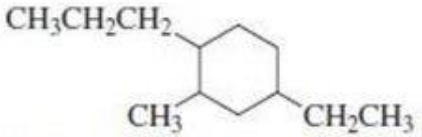


For substituted cycloalkanes, **start at a point of attachment** and number around the ring.

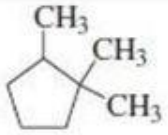
If two or more substituents are present, the substituent given the number 1 position is the one that results in a **second substituent getting as low a number** as possible.

Nomenclature of Cycloalkanes

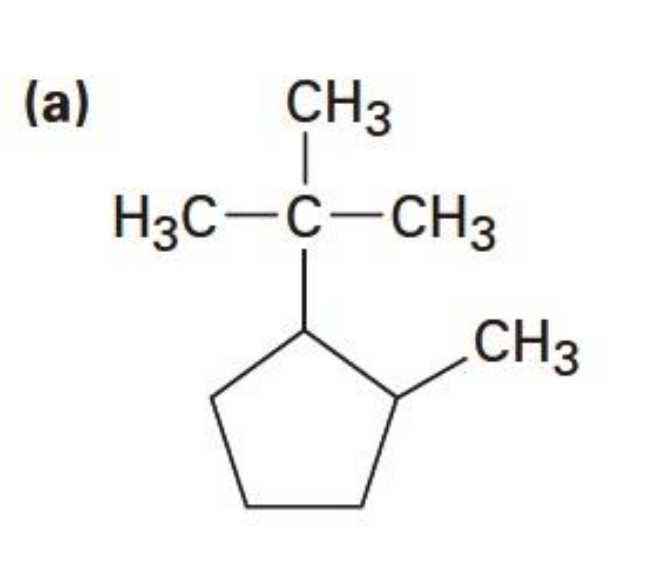
- If there are more than two substituents on the ring, they are cited in alphabetical order.
- The substituent given the number 1 position is the one that results in a second substituent getting as low a number as possible.
- If two substituents have the same low number, the ring is numbered in the direction that gives the third substituent the lowest possible number.
- Examples,



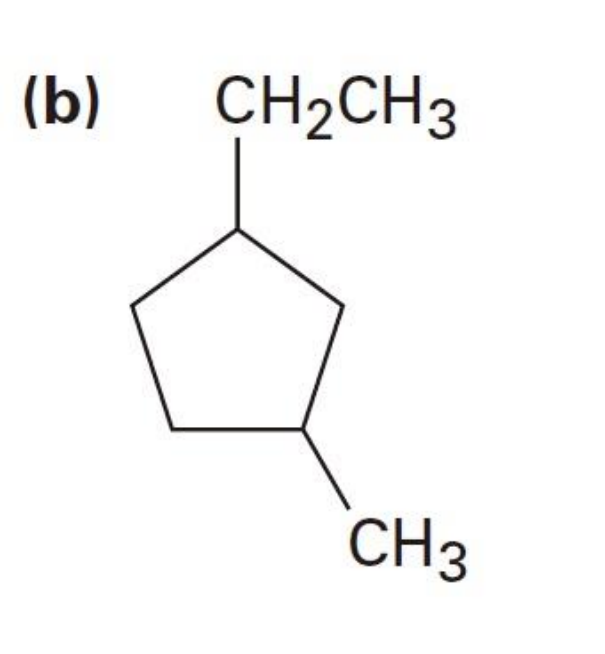
4-ethyl-2-methyl-1-propylcyclohexane
not
1-ethyl-3-methyl-4-propylcyclohexane
because 2 < 3
not
5-ethyl-1-methyl-2-propylcyclohexane
because 4 < 5



1,1,2-trimethylcyclopentane
not
1,2,2-trimethylcyclopentane
because 1 < 2
not
1,1,5-trimethylcyclopentane
because 2 < 5



(a) 1-*tert*-**B**utyl-2-**m**ethylcyclopentane



(b) 1-Ethyl-3-methylcyclopentane