WILEY

Organic Chemistry

Third Edition

David Klein

Chapter 4

Alkanes and Cycloalkanes

4.2 IUPAC Nomenclature - Alkanes

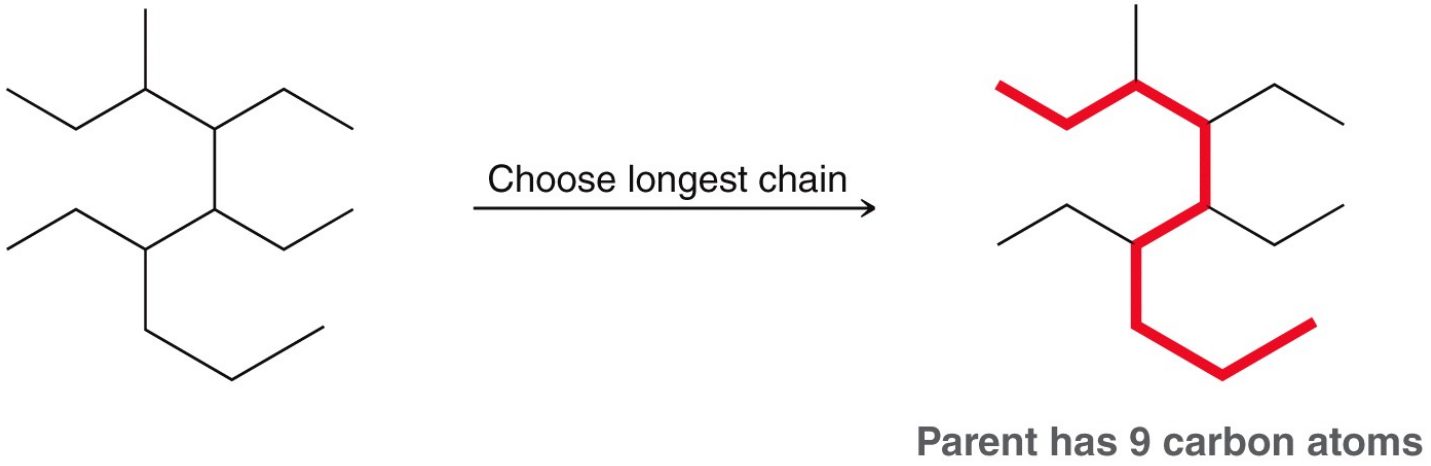
- The **IUPAC** system – **systematic** naming of compounds

- IUPAC name includes:

  - Parent name (longest carbon chain)
  - Names of substituents
  - Location of substituents

4.2 Selecting the Parent Chain

1. Identify the **parent chain** - the longest consecutive chain of carbons

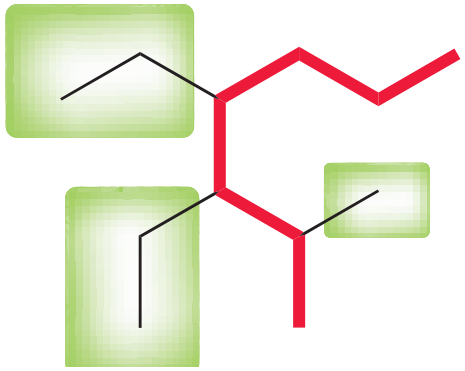


4.2 Selecting the Parent Chain

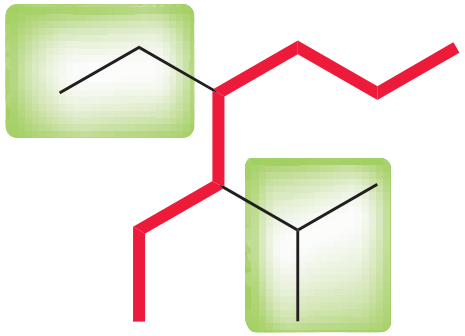
1. Identify the **parent chain** - the longest consecutive chain of carbons

If there is more than one possible parent chain, choose the one with the most substituents attached

Correct
(3 substituents)



Incorrect
(2 substituents)



4.2 Selecting the Parent Chain

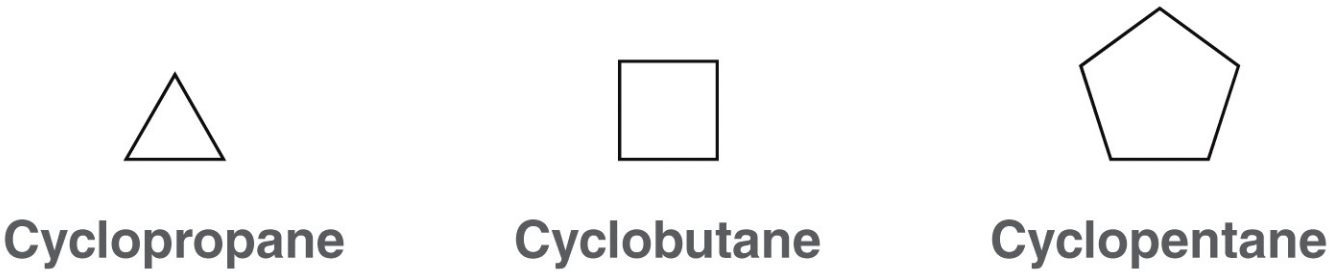
TABLE 4.1 PARENT NAMES FOR ALKANES

NUMBER OF CARBON ATOMS	PARENT	NAME OF ALKANE	NUMBER OF CARBON ATOMS	PARENT	NAME OF ALKANE
1	*meth*	methane	11	*undec*	undecane
2	*eth*	ethane	12	*dodec*	dodecane
3	*prop*	propane	13	*tridec*	tridecane
4	*but*	butane	14	*tetradec*	tetradecane
5	*pent*	pentane	15	*pentadec*	pentadecane
6	*hex*	hexane	20	*eicos*	eicosane
7	*hept*	heptane	30	*triacont*	triacontane
8	*oct*	octane	40	*tetracont*	tetracontane
9	*non*	nonane	50	*pentacont*	pentacontane
10	*dec*	decane	100	*hect*	hectane

4.2 Selecting the Parent Chain

1. Identify the **parent chain** - the longest consecutive chain of carbons

   If the parent chain is cyclic, add the prefix “cyclo”

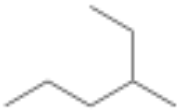


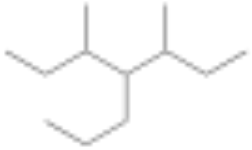
Cyclopropane Cyclobutane Cyclopentane

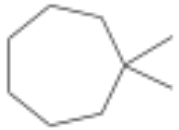
- Practice with Skillbuilder 4.1

4.2 Selecting the Parent Chain

- **Practice the Skill 4.1** – Identify and name the parent in each of the following compounds







4.2 Naming Substituents

2. Identify and name the substituents

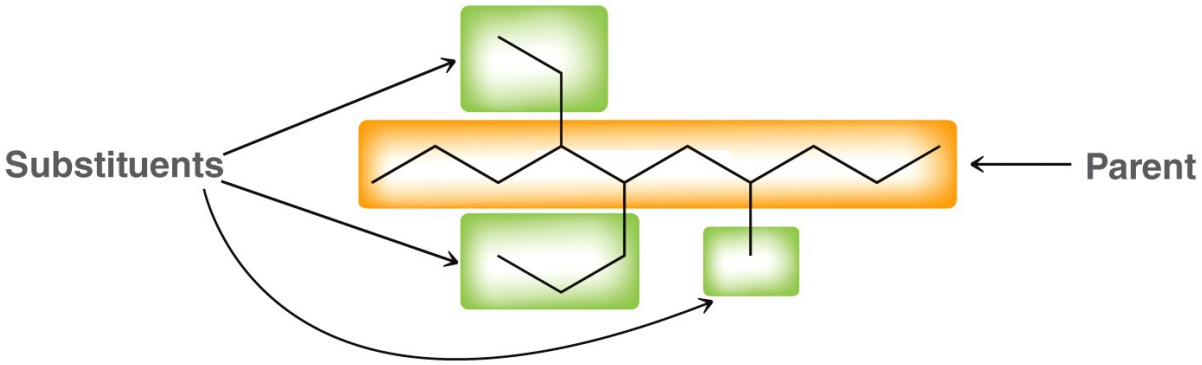
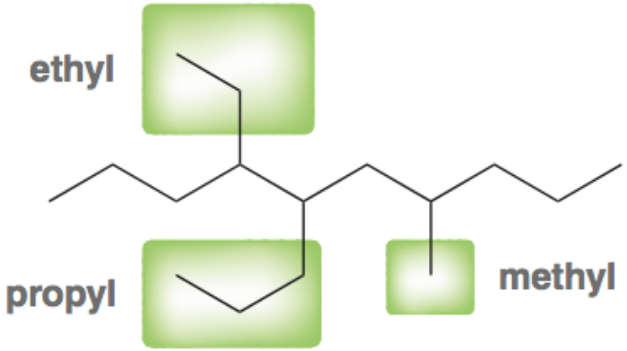


TABLE 4.2 NAMES OF ALKYL GROUPS

NUMBER OF CARBON ATOMS IN SUBSTITUENT	TERMINOLOGY
1	*methyl*
2	*ethyl*
3	*propyl*
4	*butyl*
5	*pentyl*
6	*hexyl*
7	*heptyl*
8	*octyl*
9	*nonyl*
10	*decyl*

4.2 Naming Substituents

2. Identify and name the substituents



Substituents end in yl instead of ane.

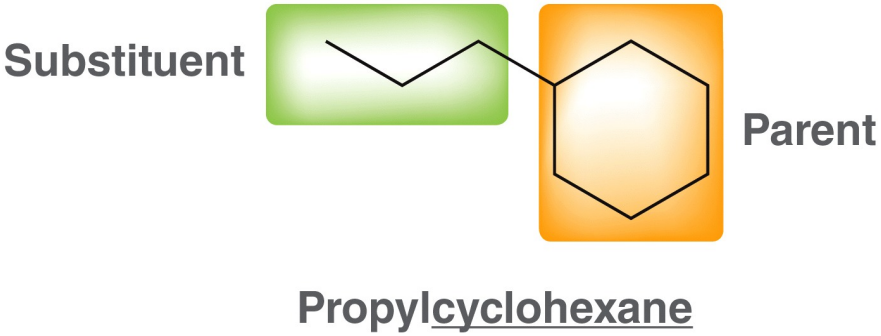
TABLE 4.2 NAMES OF ALKYL GROUPS

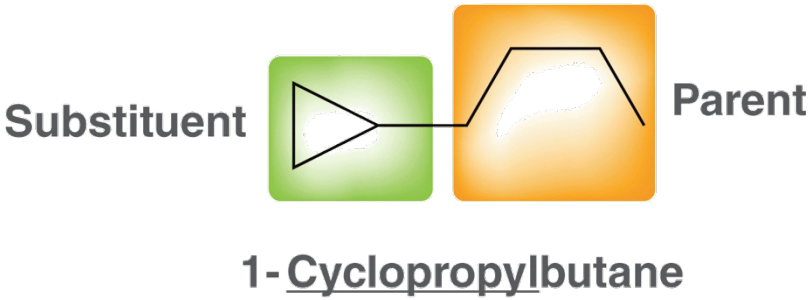
NUMBER OF CARBON ATOMS IN SUBSTITUENT	TERMINOLOGY
1	*methyl*
2	*ethyl*
3	*propyl*
4	*butyl*
5	*pentyl*
6	*hexyl*
7	*heptyl*
8	*octyl*
9	*nonyl*
10	*decyl*

4.2 Naming Substituents

2. Identify and name the substituents

A ring can be either a parent chain or a substituent depending on the number of carbons

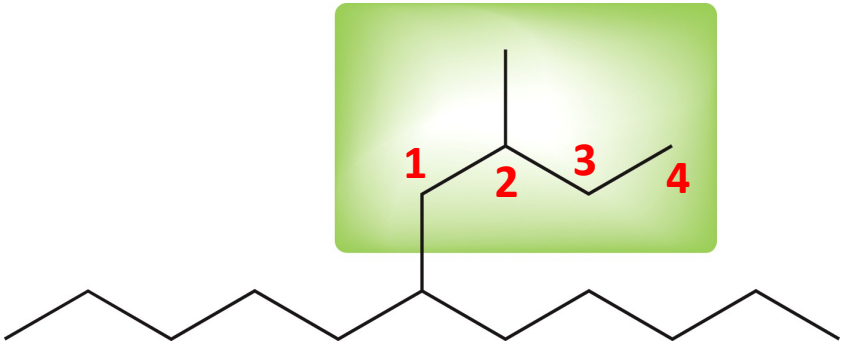




- Practice with Skillbuilder 4.2

4.2 Naming Substituents

2. Identify and name the substituents
   - For substituents with complex branches

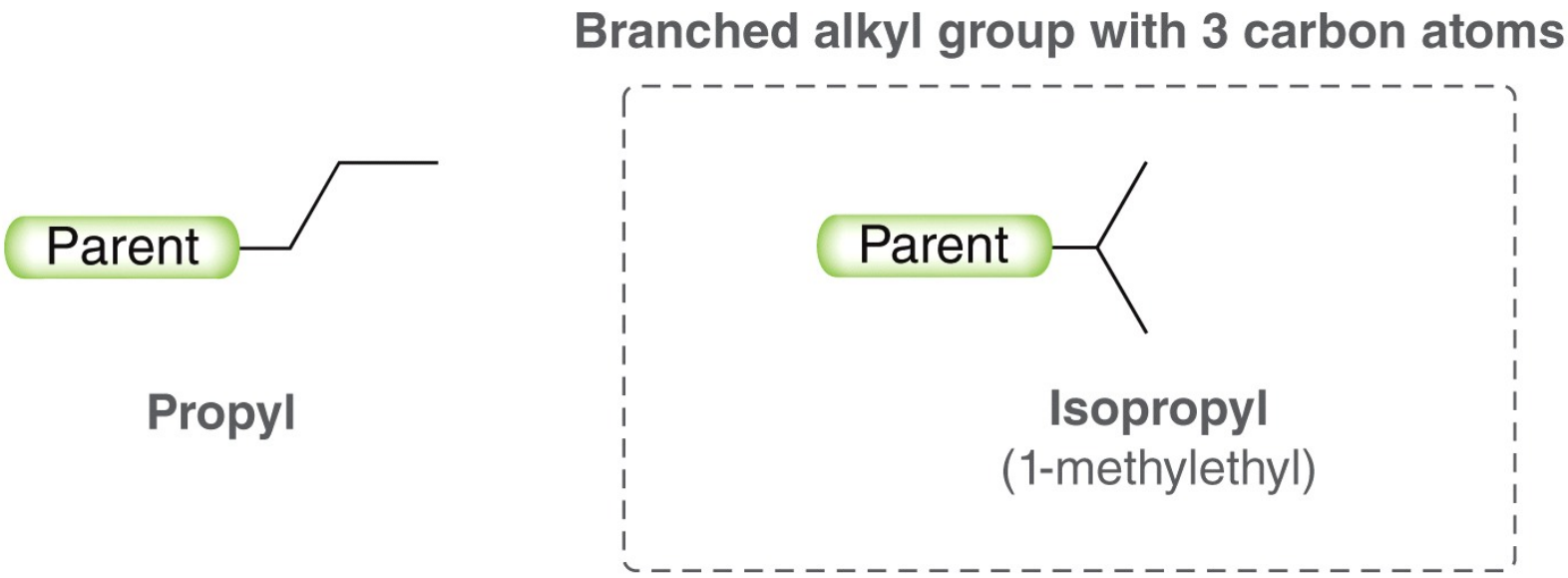


1. Number the longest carbon chain WITHIN the substituent. Start with the carbon attached to the parent chain
2. Name the substituent (in this case butyl)
3. Name and Number the substituent's side group (in this case 2-methyl)

   The name of the substituent is **(2-methylbutyl)**

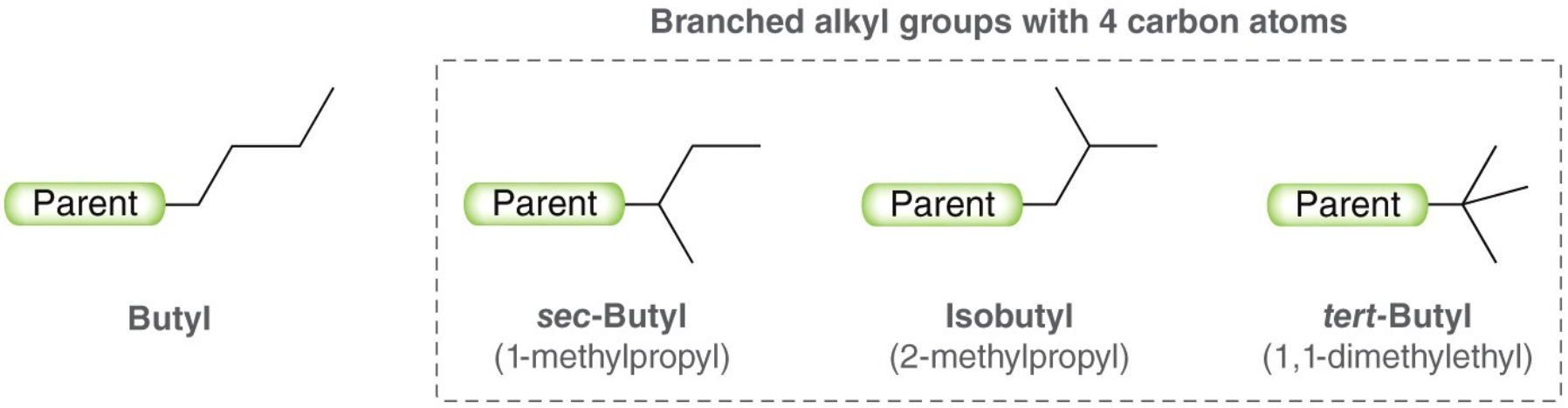
4.2 Naming Substituents

2. Identify and name the substituents
   - Some branched substituents have **common** names
   - Two types of propyl groups



4.2 Naming Substituents

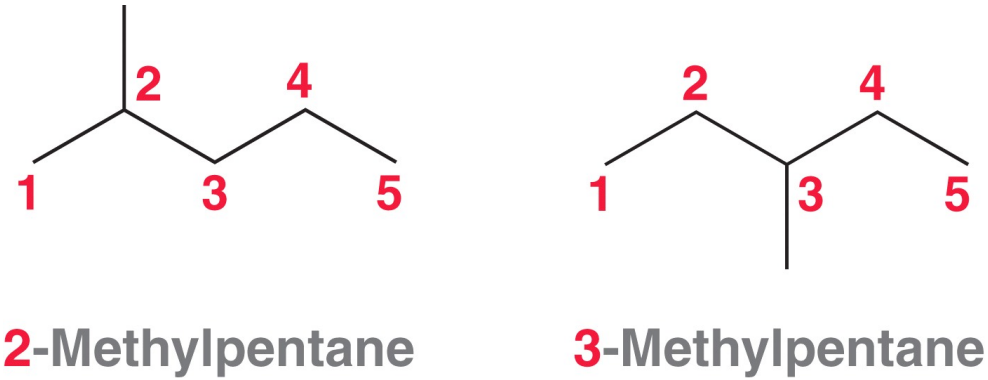
2. Identify and name the substituents
   - Some branched substituents have **common** names
   - Three types of butyl groups



- Practice with Skillbuilder 4.3

4.2 Assembling the IUPAC Name

- Carbons in the parent chain have to be **numbered**

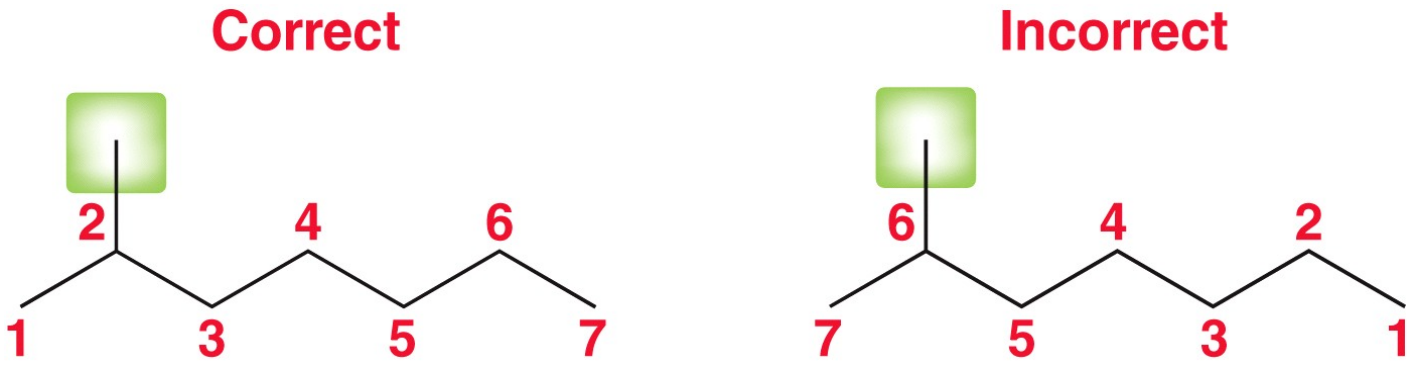


- **2-methyl**pentane means there is a **methyl** group on **carbon #2** of the pentane chain

4.2 Assembling the IUPAC Name

- Guidelines to follow when numbering the parent chain

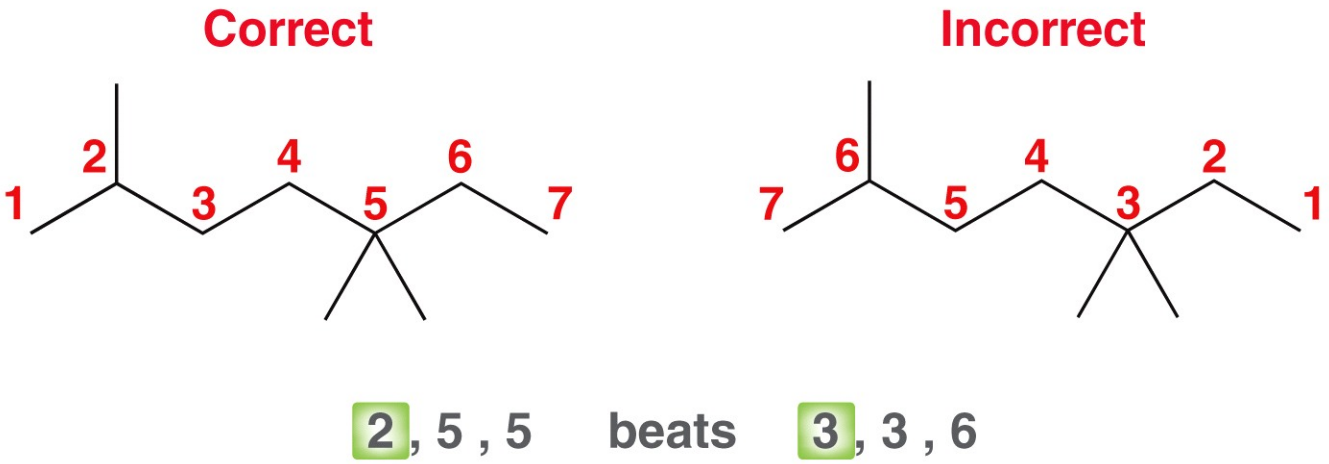
1. If ONE substituent is present, number the parent chain so that the substituent has the lowest number possible



4.2 Assembling the IUPAC Name

- Guidelines to follow when numbering the parent chain

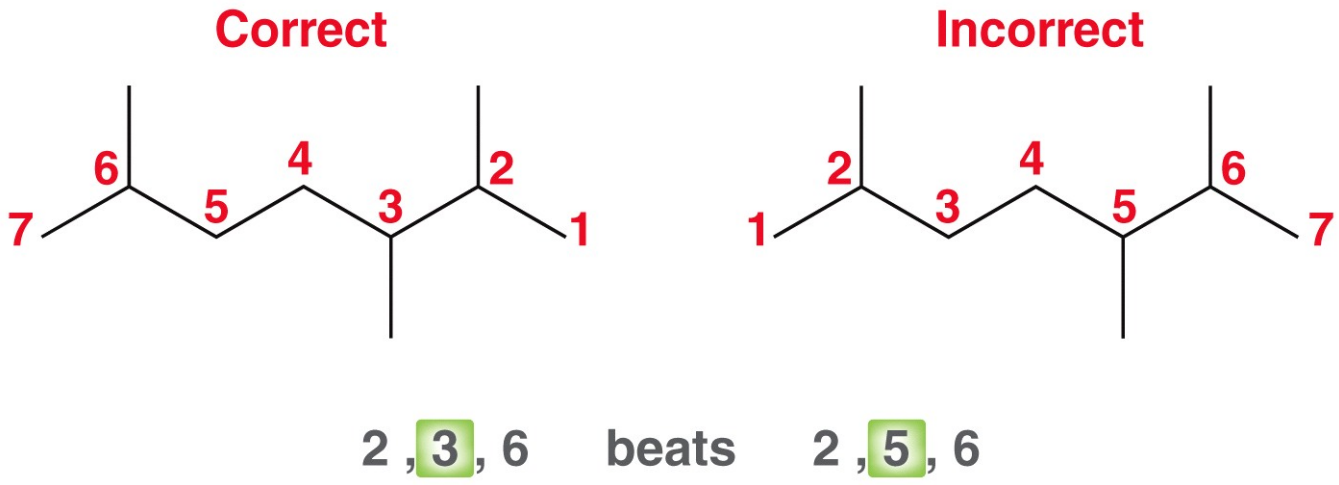
2. When multiple substituents are present, number the parent chain to give the first substituent the lowest number possible



4.2 Assembling the IUPAC Name

- Guidelines to follow when numbering the parent chain

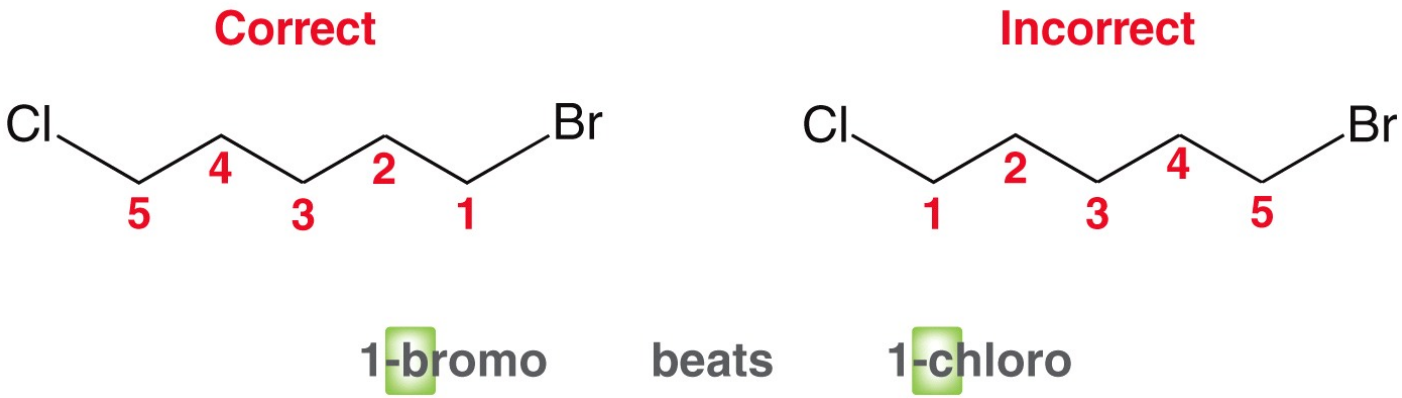
3. If there is a tie, then number the parent chain so that the second locant gets the lowest number possible



4.2 Assembling the IUPAC Name

- Guidelines to follow when numbering the parent chain

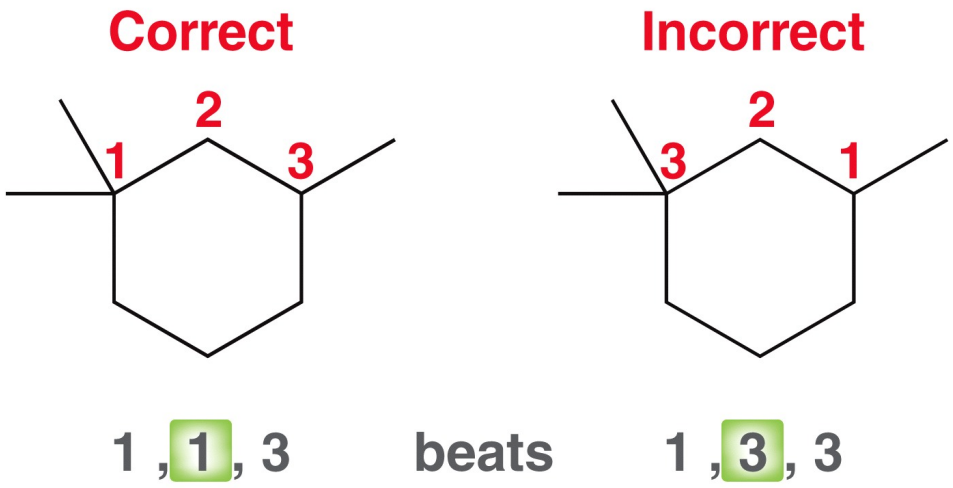
4. If there is no other tie-breaker, then assign the lowest number alphabetically



4.2 Assembling the IUPAC Name

- Guidelines to follow when numbering the parent chain

  – The same rules apply for cycloalkanes



4.2 Assembling the IUPAC Name

To assemble the complete name:

1. Put the # and name of each substituent before the parent chain name, ***in alphabetical order***

5. A prefix is used (di, tri, tetra, penta, etc.) if multiple substituents are identical.

note: “di” or “tri” is ignored when alphabetizing the substituents

4.2 IUPAC Rules - Summary

1. **Identify the parent chain**

2. **Identify and Name the substituents**

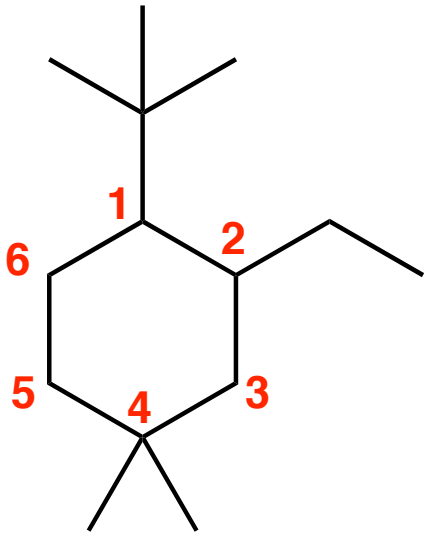
3. **Number the parent chain; assign a locant to each substituent**

4. **List the numbered substituents before the parent name in alphabetical order**

- Practice with SkillBuilder 4.4

4.2 IUPAC Rules - Summary

- Following the rules, we can name the following compound:



Parent name:

cyclohexane

Substituents:

1-*tert*-butyl

2-ethyl

4-methyl

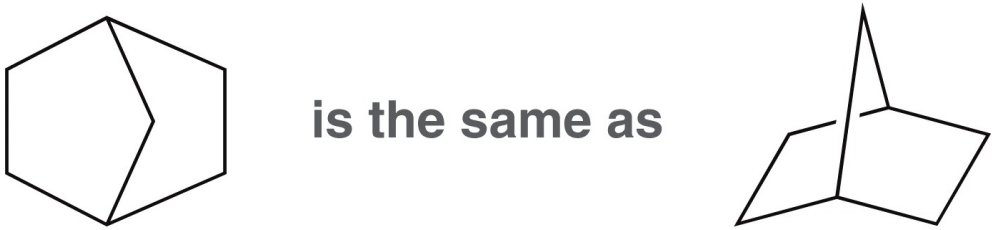
4-methyl

4,4-dimethyl

1-*tert*-butyl-2-ethyl-4,4-dimethylcyclohexane

4.2 Naming Bicyclic Compounds

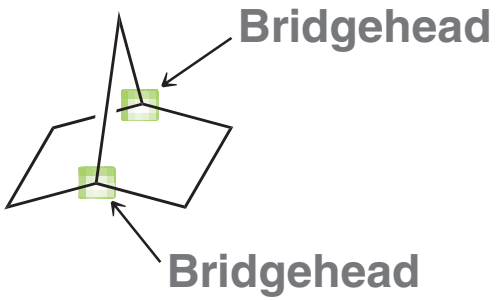
- **Bicyclic** compound contains two fused rings.



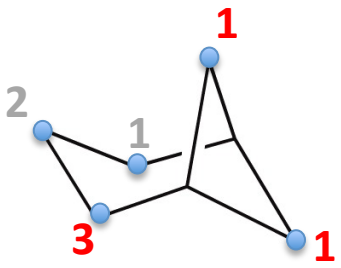
- To name a bicyclic compound, include the prefix **bicyclo** in front of the parent name

4.2 Naming Bicyclic Compounds

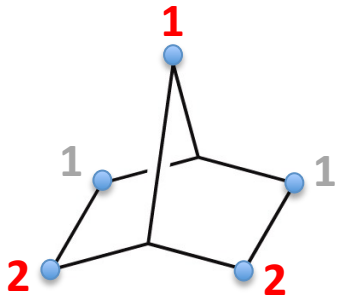
- The two carbons where the rings are fused are **bridgehead** carbons



- There are three "paths" connecting the bridgeheads. Count the number of carbons in each path to name the compound



Bicyclo[3.1.1]heptane



Bicyclo[2.2.1]heptane

- Practice with Skillbuilder 4.5

4.3 Constitutional Isomers

- **ISOMERS**
  - different structures, same molecular formula

- **CONSTITUTIONAL ISOMERS**
  - different connectivity of atoms

4.3 Constitutional Isomers

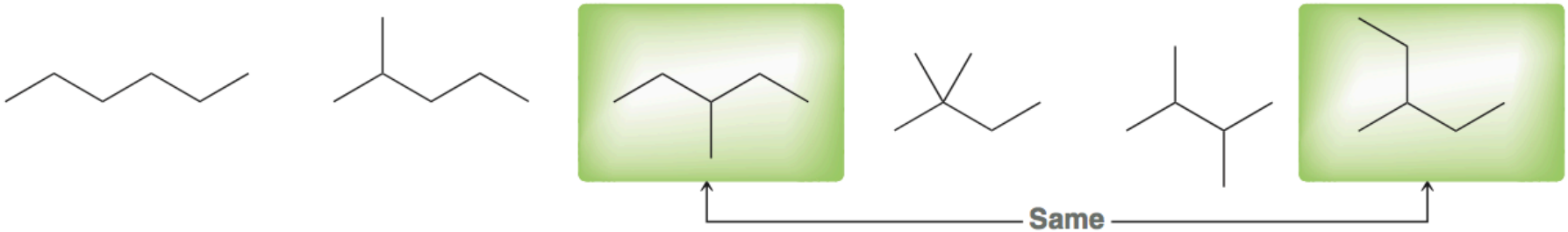
- As the number of carbon atoms increases, the number of constitutional isomers increases

TABLE 4.4 NUMBER OF CONSTITUTIONAL ISOMERS FOR VARIOUS ALKANES

MOLECULAR FORMULA	NUMBER OF CONSTITUTIONAL ISOMERS
C_3H_8	1
C_4H_{10}	2
C_5H_{12}	3
C_6H_{14}	5
C_7H_{16}	9
C_8H_{18}	18
C_9H_{20}	35
$C_{10}H_{22}$	75
$C_{15}H_{32}$	4,347
$C_{20}H_{42}$	366,319
$C_{30}H_{62}$	4,111,846,763
$C_{40}H_{82}$	62,481,801,147,341

4.3 Constitutional Isomers

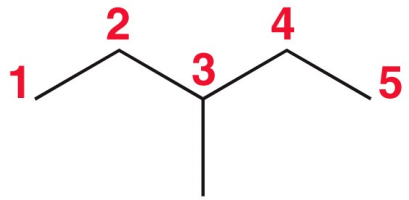
- Be able to recognize different structures as either being isomers, or being the same compound.



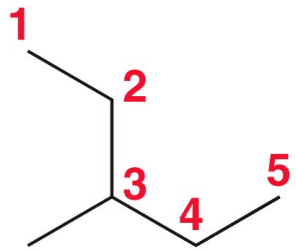
- You can test if structures are the same in two ways:
  1. Flip one of the molecules in 3D space and rotate around its single bonds until it is super-imposable on the other molecule
  2. Name them. If they have the same IUPAC name, they are the same compound

4.3 Constitutional Isomers

180˚ rotation along the C3 – C4 bond would make it more obvious these two compounds are the same



3-Methylpentane



3-Methylpentane

- Following IUPAC rules for naming yields the same name as well
- Practice with SkillBuilder 4.6