3.4: CYCLOALKANES

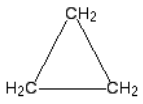
learning objectives

- name cycloalkanes using IUPAC (systematic) and selected common name nomenclature
- draw the structure of cycloalkanes from IUPAC (systematic) and selected common names

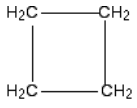
Cycloalkanes are cyclic hydrocarbons, meaning that the carbons of the molecule are arranged in the form of a ring. Cycloalkanes are also saturated, meaning that all of the carbons atoms that make up the ring are single bonded to other atoms (no double or triple bonds). There are also polycyclic alkanes, which are molecules that contain two or more cycloalkanes that are joined, forming multiple rings.

INTRODUCTION

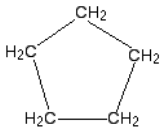
Many organic compounds found in nature or created in a laboratory contain rings of carbon atoms with distinguishing chemical properties; these compounds are known as cycloalkanes. Cycloalkanes only contain carbon-hydrogen bonds and carbon-carbon single bonds, but in cycloalkanes, the carbon atoms are joined in a ring. The smallest cycloalkane is cyclopropane.



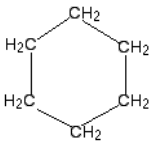
cyclopropane



cyclobutane



cyclopentane



cyclohexane

If you count the carbons and hydrogens, you will see that they no longer fit the general formula C_nH_{2n+2}. By joining the carbon atoms in a ring,two hydrogen atoms have been lost. The general formula for a cycloalkane is C_nH_{2n}. Cyclic compounds are not all flat molecules. All of the cycloalkanes, from cyclopentane upwards, exist as "puckered rings". Cyclohexane, for example, has a ring structure that looks like this:

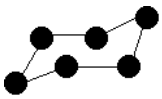
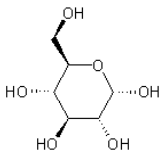
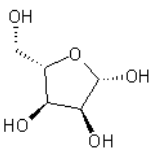


Figure 2: This is known as the "chair" form of cyclohexane from its shape, which vaguely resembles a chair. Note: The cyclohexane molecule is constantly changing, with the atom on the left, which is currently pointing down, flipping up, and the atom on the right flipping down. During this process, another (slightly less stable) form of cyclohexane is formed known as the "boat" form. In this arrangement, both of these atoms are either pointing up or down at the same time

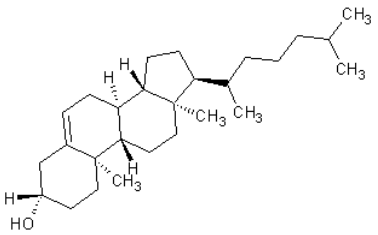
In addition to being saturated cyclic hydrocarbons, cycloalkanes may have multiple substituents or functional groups that further determine their unique chemical properties. The most common and useful cycloalkanes in organic chemistry are cyclopentane and cyclohexane, although other cycloalkanes varying in the number of carbons can be synthesized. Understanding cycloalkanes and their properties are crucial in that many of the biological processes that occur in most living things have cycloalkane-like structures.



Glucose (6 carbon sugar)



Ribose (5 carbon sugar)

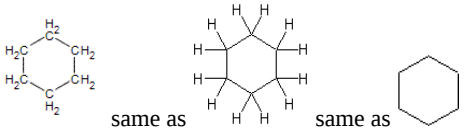


Cholesterol (polycyclic)

Although polycyclic compounds are important, they are highly complex and typically have common names accepted by IUPAC. However, the common names do not generally follow the basic IUPAC nomenclature rules. The general formula of the cycloalkanes is C_nH_{2n} where n is the number of carbons. The naming of cycloalkanes follows a simple set of rules that are built upon the same basic steps in naming alkanes. Cyclic hydrocarbons have the prefix "cyclo-".

CONTENTS

For simplicity, cycloalkane molecules can be drawn in the form of skeletal structures in which each intersection between two lines is assumed to have a carbon atom with its corresponding number of hydrogens.



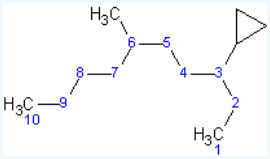
Cycloalkane	Molecular Formula	Basic Structure
Cyclopropane	C_3H_6	
Cyclobutane	C_4H_8	
Cyclopentane	C_5H_{10}	
Cyclohexane	C_6H_{12}	
Cycloheptane	C_7H_{14}	
Cyclooctane	C_8H_{16}	
Cyclononane	C_9H_{18}	
Cyclodecane	$C_{10}H_{20}$	

IUPAC RULES FOR NOMENCLATURE

1. Determine the cycloalkane to use as the parent chain. The parent chain is the one with the highest number of carbon atoms. If there are two cycloalkanes, use the cycloalkane with the higher number of carbons as the parent chain.
2. If there is an alkyl straight chain that has a greater number of carbons than the cycloalkane, then the alkyl chain must be used as the primary parent chain. Cycloalkane acting as a substituent to an alkyl chain has an ending "-yl" and, therefore, must be named as a cycloalkyl.

Cycloalkane	Cycloalkyl
cyclopropane	cyclopropyl
cyclobutane	cyclobutyl
cyclopentane	cyclopentyl
cyclohexane	cyclohexyl
cycloheptane	cycloheptyl
cyclooctane	cyclooctyl
cyclononane	cyclononanyl
cyclodecane	cyclodecanyl

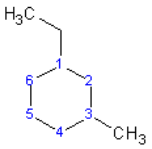
Example 3.4.1:



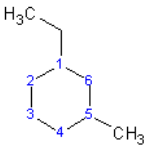
The longest straight chain contains 10 carbons, compared with cyclopropane, which only contains 3 carbons. Because cyclopropane is a substituent, it would be named a cyclopropyl-substituted alkane.

3) Determine any functional groups or other alkyl groups.

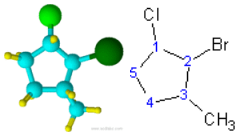
4) Number the carbons of the cycloalkane so that the carbons with functional groups or alkyl groups have the lowest possible number. A carbon with multiple substituents should have a lower number than a carbon with only one substituent or functional group. One way to make sure that the lowest number possible is assigned is to number the carbons so that when the numbers corresponding to the substituents are added, their sum is the lowest possible.



1-ethyl-3-methylcyclohexane (1+3=4) **NOT** 1-ethyl-5-methylcyclohexane (1+5=6)



5) When naming the cycloalkane, the substituents and functional groups must be placed in alphabetical order.



(ex: 2-bromo-1-chloro-3-methylcyclopentane)

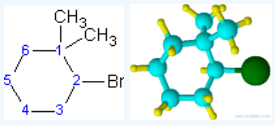
6) Indicate the carbon number with the functional group with the highest priority according to alphabetical order. A dash"-" must be placed between the numbers and the name of the substituent. After the carbon number and the dash, the name of the substituent can follow. When there is only one substituent on the parent chain, indicating the number of the carbon atoms with the substituent is not necessary.

(ex: 1-chlorocyclohexane or cholorocyclohexane is acceptable)

7) If there is more than one of the same functional group on one carbon, write the number of the carbon two, three, or four times, depending on how many of the same functional group is present on that carbon. The numbers must be separated by commas, and the name of the functional group that follows must be separated by a dash. When there are two of the same functional group, the name must have the prefix "di". When there are three of the same functional group, the name must have the prefix "tri". When there are four of the same functional group, the name must have the prefix "tetra". However, these prefixes cannot be used when determining the alphabetical priorities.

There must always be commas between the numbers and the dashes that are between the numbers and the names.

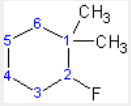
Example 3.4.2



(2-bromo-1,1-dimethylcyclohexane)

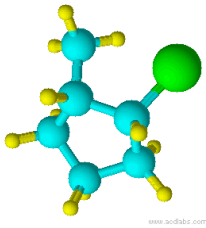
Notice that "f" of fluoro alphabetically precedes the "m" of methyl. Although "di" alphabetically precedes "f", it is not used in determining the alphabetical order.

Example 3



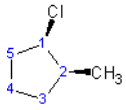
(2-fluoro-1,1,-dimethylcyclohexane **NOT** 1,1-dimethyl-2-fluorocyclohexane)

8) If the substituents of the cycloalkane are related by the cis or trans configuration, then indicate the configuration by placing "cis-" or "trans-" in front of the name of the structure.



Blue=Carbon Yellow=Hydrogen Green=Chlorine

Notice that chlorine and the methyl group are both pointed in the same direction on the axis of the molecule; therefore, they are cis.



cis-1-chloro-2-methylcyclopentane

9) After all the functional groups and substituents have been mentioned with their corresponding numbers, the name of the cycloalkane can follow.

SUMMARY

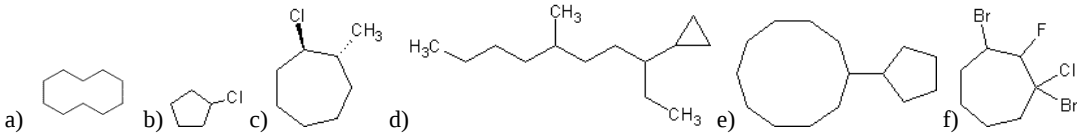
1. Determine the parent chain: the parent chain contains the most carbon atoms.
2. Number the substituents of the chain so that the sum of the numbers is the lowest possible.
3. Name the substituents and place them in alphabetical order.
4. If stereochemistry of the compound is shown, indicate the orientation as part of the nomenclature.
5. Cyclic hydrocarbons have the prefix "cyclo-" and have an "-alkane" ending unless there is an alcohol substituent present. When an alcohol substituent is present, the molecule has an "-ol" ending.

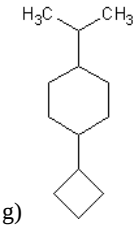
GLOSSARY

- **alkyl:** A structure that is formed when a hydrogen atom is removed from an alkane.
- **cyclic:** Chemical compounds arranged in the form of a ring or a closed chain form.
- **cycloalkanes:** Cyclic saturated hydrocarbons with a general formula of CnH(2n). Cycloalkanes are alkanes with carbon atoms attached in the form of a closed ring.
- **functional groups:** An atom or groups of atoms that substitute for a hydrogen atom in an organic compound, giving the compound unique chemical properties and determining its reactivity.
- **hydrocarbon:** A chemical compound containing only carbon and hydrogen atoms.
- **saturated**: All of the atoms that make up a compound are single bonded to the other atoms, with no double or triple bonds.
- **skeletal structure:** A simplified structure in which each intersection between two lines is assumed to have a carbon atom with its corresponding number of hydrogens.

EXERCISES

1. Name the following structures. (Note: The structures are complex for practice purposes and may not be found in nature.)





g)

2. Draw the following structures.

a) 1,1-dibromo-5-fluoro-3-butyl-7-methylcyclooctane

b) trans-1-bromo-2-chlorocyclopentane

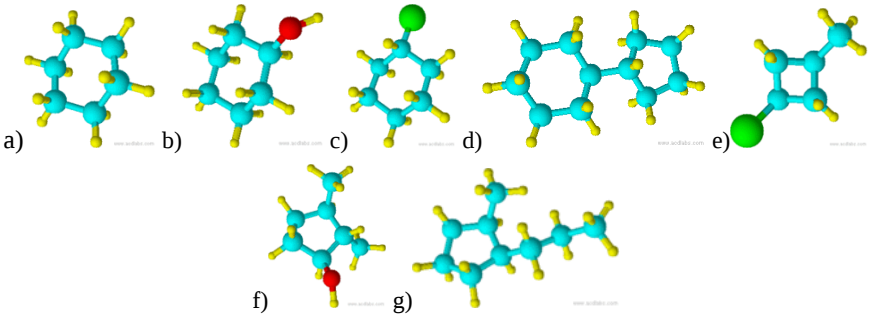
c) 1,1-dibromo-2,3-dichloro-4-propylcyclobutane

d) 2-methyl-1-ethyl-1,3-dipropylcyclopentane

e) cycloheptane-1,3,5-triol

3. Name the following structures.

Blue=Carbon Yellow=Hydrogen Red=Oxygen Green=Chlorine



a) b) c) d) e)

f) g)

SOLUTIONS

1. a) cyclodecane

b) chlorocyclopentane or 1-chlorocyclopentane

c) trans-1-chloro-2-methylcycloheptane

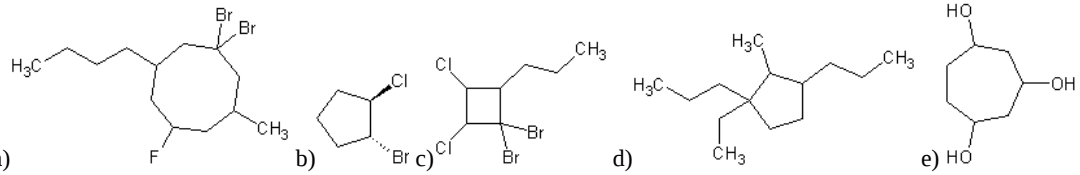
d) 3-cyclopropyl-6-methyldecane

e) cyclopentylcyclodecane or 1-cyclopentylcyclodecane

f) 1,3-dibromo-1-chloro-2-fluorocycloheptane

g) 1-cyclobutyl-4-isopropylcyclohexane

2.



a) b) c) d) e)

3. a) cyclohexane

b) cyclohexanol

c) chlorocyclohexane

d) cyclopentylcyclohexane

e) 1-chloro-3-methylcyclobutane

f) 2,3-dimethylcyclohexanol

g) cis-1-propyl-2-methylcyclopentane

REFERENCES

1. ACD/ChemSketch Freeware, version 11.0, Advanced Chemistry Development, Inc., Toronto, ON, Canada, www.acdlabs.com, 2008.
2. Bruice, Paula Yurkanis. Oragnic Chemistry. 5th. CA. Prentice Hall, 2006.
3. Fryhle, C.B. and G. Solomons. Organic Chemistry. 9th ed. Danvers, MA: Wiley, 2008.
4. McMurry, John. Organic Chemistry. 7th ed. Belmont, California: Thomson Higher Education, 2008.
5. Sadava, Heller, Orians, Purves, Hillis. Life The Science of Biology. 8th ed. Sunderland, MA: W.H. Freeman, 2008.
6. Vollhardt, K. Peter C., and Neil E. Schore. Organic Chemistry. 5th ed. New York: W.H. Freeman, 2007.

CONTRIBUTORS AND ATTRIBUTIONS

- Pwint Zin
- Jim Clark (ChemGuide)
