Objectives

After completing this section, you should be able to

1. name a substituted or unsubstituted cycloalkane, given its Kekulé structure, shorthand structure or condensed structure.
2. draw the Kekulé, shorthand or condensed structure for a substituted or unsubstituted cycloalkane, given its IUPAC name.

Key Terms

Make certain that you can define, and use in context, the key terms below.

- cycloalkane

Study Notes

Provided that you have mastered the IUPAC system for naming alkanes, you should find that the nomenclature of cycloalkanes does not present any particular difficulties.

Many organic compounds found in nature contain rings of carbon atoms. These compounds are known as cycloalkanes. **Cycloalkanes** have one or more rings of carbon atoms. Cycloalkanes only contain carbon-hydrogen bonds and carbon-carbon single bonds. The simplest examples of this class consist of a single, un-substituted carbon ring, and these form a homologous series similar to the unbranched alkanes.

Like alkanes, cycloalkane molecules are often drawn as skeletal structures in which each intersection between two lines is assumed to have a carbon atom with its corresponding number of hydrogens. Cyclohexane, one of the most common cycloalkanes is shown below as an example.
Cyclic hydrocarbons have the prefix "cyclo-". The IUPAC names, molecular formulas, and skeleton structures of the first ten cycloalkanes are given in Table 4.1.1. Note that the general formula for a cycloalkane composed of \( n \) carbons is \( C_nH_{2n} \), and not \( C_nH_{2n+2} \) as for alkanes. Although a cycloalkane has two fewer hydrogens than the equivalent alkane, each carbon is bonded to four other atoms so are still considered to be saturated with hydrogen.

<table>
<thead>
<tr>
<th>Cycloalkane</th>
<th>Molecular Formula</th>
<th>Skeleton Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cyclopropane</td>
<td>C(_3)H(_6)</td>
<td><img src="structure.png" alt="Cyclopropane Structure" /></td>
</tr>
<tr>
<td>Cyclobutane</td>
<td>C(_4)H(_8)</td>
<td><img src="structure.png" alt="Cyclobutane Structure" /></td>
</tr>
<tr>
<td>Cyclopentane</td>
<td>C(<em>5)H(</em>{10})</td>
<td><img src="structure.png" alt="Cyclopentane Structure" /></td>
</tr>
<tr>
<td>Cyclohexane</td>
<td>C(<em>6)H(</em>{12})</td>
<td><img src="structure.png" alt="Cyclohexane Structure" /></td>
</tr>
<tr>
<td>Cycloheptane</td>
<td>C(<em>7)H(</em>{14})</td>
<td><img src="structure.png" alt="Cycloheptane Structure" /></td>
</tr>
<tr>
<td>Cyclooctane</td>
<td>C(<em>8)H(</em>{16})</td>
<td><img src="structure.png" alt="Cyclooctane Structure" /></td>
</tr>
<tr>
<td>Cyclononane</td>
<td>C(<em>9)H(</em>{18})</td>
<td><img src="structure.png" alt="Cyclononane Structure" /></td>
</tr>
</tbody>
</table>
### Table 4.1.1: Examples of Simple Cycloalkanes

<table>
<thead>
<tr>
<th>Cycloalkane</th>
<th>Molecular Formula</th>
<th>Skeleton Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cyclooctane</td>
<td>C&lt;sub&gt;10&lt;/sub&gt;H&lt;sub&gt;20&lt;/sub&gt;</td>
<td>![Cyclooctane Skeleton]</td>
</tr>
</tbody>
</table>

IUPAC Rules for Nomenclature

The naming of substituted cycloalkanes follows the same basic steps used in naming alkanes.

1. Determine the parent chain.
2. Number the substituents of the ring so that the sum of the numbers is the lowest possible.
3. Name the substituents and place them in alphabetical order.

More specific rules for naming substituted cycloalkanes with examples are given below.

1. Determine the cycloalkane to use as the parent. 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. Cycloalkanes substituents have an ending "-yl". If there are two cycloalkanes in the molecule, use the cycloalkane with the higher number of carbons as the parent.

Example 4.1.1

![Example Molecule]

The longest straight chain contains 10 carbons, compared with cyclopropane, which only contains 3 carbons. The parent chain in this molecule is decane and cyclopropane is a substituent. The name of this molecule is 3-cyclopropyl-3,10-dimethyldecane.
2) When there is only one substituent on the ring, the ring carbon attached to the substituent is automatically carbon #1. Indicating the number of the carbon with the substituent in the name is optional.

Example 4.1.2

1-chlorocyclobutane or chlorocyclobutane 1-propylcyclohexane or propylcyclohexane

If there are multiple substituents on the ring, number the carbons of the cycloalkane so that the carbons with substituents 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.

Example 4.1.3

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

3) When naming the cycloalkane, the substituents must be placed in alphabetical order. Remember the prefixes di-, tri-, etc., are not used for alphabetization.

Example 4.1.4
2-bromo-1-chloro-3-methylcyclopentane

Notice that "f" of fluoro alphabetically precedes the "m" of methyl.

Example 4.1.5

(2-bromo-1,1-dimethylcyclohexane)

Although "di" alphabetically precedes "f", "di" is not used in determining the alphabetical order.

Example 4.1.6

(2-fluoro-1,1-dimethylcyclohexane NOT 1,1-dimethyl-2-fluorocyclohexane)
Hydrocarbons having more than one ring are common, and are referred to as **bicyclic** (two rings), **tricyclic** (three rings) and in general, **polycyclic** compounds. The molecular formulas of such compounds have H/C ratios that decrease with the number of rings. In general, for a hydrocarbon composed of \( n \) carbon atoms associated with \( m \) rings the formula is: \( C_nH(2n + 2 - 2m) \). The structural relationship of rings in a polycyclic compound can vary. They may be separate and independent, or they may share one or two common atoms. Some examples of these possible arrangements are shown in the following table.

<table>
<thead>
<tr>
<th>Isolated Rings</th>
<th>Spiro Rings</th>
<th>Fused Rings</th>
<th>Bridged Rings</th>
</tr>
</thead>
<tbody>
<tr>
<td>No common atoms</td>
<td>One common atom</td>
<td>One common bond</td>
<td>Two common atoms</td>
</tr>
</tbody>
</table>

![Diagram of polycyclic compounds](image)

Polycyclic compounds, like cholesterol shown below, are biologically important and typically have common names accepted by IUPAC. However, the common names do not generally follow the basic IUPAC nomenclature rules, and will not be covered here.
Problems

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

1)

2)

3)

4)

5)

6)
Draw the following structures.

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

8) 1,1-dibromo-2,3-dichloro-4-propylcyclobutane

9) 1-ethyl-2-methyl-1,3-dipropylcyclopentane

Name the following structures.

Blue = Carbon  Yellow = Hydrogen  Green = Chlorine
Answers to Practice Problems

1) cyclodecane 2) chlorocyclopentane or 1-chlorocyclopentane

3) 6-methyl-3-cyclopropyldecane 4) cyclopentylcyclodecane or 1-cyclopentylcyclodecane 5) 1,3-dibromo-1-chloro-2-fluorocycloheptane

6) 1-cyclobutyl-4-isopropylcyclohexane

7) $\text{H}_3\text{C} - \text{Br} \quad \text{Br} \quad \text{Br}$

8) $\text{Cl} \quad \text{CH}_3 \quad \text{Cl} \quad \text{Br} \quad \text{Br}$

9) $\text{H}_3\text{C} \quad \text{H}_3\text{C} \quad \text{CH}_3 \quad \text{CH}_3 \quad \text{CH}_3$

10) cyclohexane 11) chlorocyclohexane 12) cyclopentylcyclohexane 13) 1-chloro-3-methylcyclobutane
Outside links

- More Practice Problems on Nomenclature of Cycloalkanes
- Wikipedia: Cycloalkanes
- http://www.cem.msu.edu/~reusch/VirtualText/nomen1.htm
- http://www.chemguide.co.uk/organicprops/alkanes/background.html
- http://www.cem.msu.edu/~reusch/VirtualText/nomen1.htm
- http://science.csustan.edu/nhuy/chem...IVNamecyal.htm
- http://en.wikibooks.org/wiki/Organic...s/Cycloalkanes

References


Exercises

Questions

Q4.1.1

Name the following compounds:
Q4.1.2

Draw the following structures

1 = 1,2-dimethylcyclohexane
2 = 2-cyclopropyl butane
3 = 1,2,3-trimethyl cyclopentane

Solutions

S4.1.1

1 = 1-cyclopropyl cyclopropane
2 = 1-isopropyl cyclohexane
3 = 2-propenyl cyclopentane
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Objectives

After completing this section, you should be able to

1. draw structural formulas that distinguish between cis and trans disubstituted cycloalkanes.
2. construct models of cis and trans disubstituted cycloalkanes using ball-and-stick molecular models.

Key Terms

Make certain that you can define, and use in context, the key terms below.

- constitutional isomer
Previously, constitutional isomers were defined as molecules that had the same molecular formula, but different atom connectivity. In this section, a new class of isomers, stereoisomers, will be introduced. **Stereoisomers** are molecules that have the same molecular formula, the same atom connectivity, but they differ in the relative spatial orientation of the atoms.

Di-substituted cycloalkanes are one class of molecules that exhibit stereoisomerism. 1,2-dibromocyclopentane can exist as two different stereoisomers: cis-1,2-dibromocyclopentane and trans-1,2-dibromocyclopentane. The cis-1,2-dibromocyclopentane and trans-1,2-dibromocyclopentane stereoisomers of 1,2-dibromocyclopentane are shown below. Both molecules have the same molecular formula and the same atom connectivity. They differ only in the relative spatial orientation of the two bromines on the ring. In cis-1,2-dibromocyclopentane, both bromine atoms are on the same "face" of the cyclopentane ring, while in trans-1,2-dibromocyclopentane, the two bromines are on opposite faces of the ring. Stereoisomers require an additional nomenclature prefix be added to the IUPAC name in order to indicate their spatial orientation. Di-substituted cycloalkane stereoisomers are designated by the nomenclature prefixes **cis** (Latin, meaning on this side) and **trans** (Latin, meaning across).

![ cis-1,2-dibromocyclopentane and trans-1,2-dibromocyclopentane stereoisomers](image)

By convention, chemists use heavy, wedge-shaped bonds to indicate a substituent located above the average plane of the ring (coming out of the page), a dashed line for bonds to atoms or groups located below the ring (going back into the page), and solid lines for bonds in the plane of the page.
In general, if any two \( sp^3 \) carbons in a ring have two different substituent groups (not counting other ring atoms) cis/trans stereoisomerism is possible. However, the cis/trans designations are not used if both groups are on the same carbon. For example, the chlorine and the methyl group are on the same carbon in 1-chloro-1-methylcyclohexane and the trans prefix should not be used.

If more than two ring carbons have substituents, the stereochemical notation distinguishing the various isomers becomes more complex and the prefixes \textit{cis} and \textit{trans} cannot be used to formally name the molecule. However, the relationship of any two substituents can be informally described using \textit{cis} or \textit{trans}. For example, in the tri-substituted cyclohexane below, the methyl group is \textit{cis} to the ethyl group, and also \textit{trans} to the chlorine. However, the entire molecule cannot be designated as either a \textit{cis} or \textit{trans} \textit{isomer}. Later sections will describe how to name these more complex molecules (5.5: \textit{Sequence Rules for Specifying Configuration}).
Exercises

Questions

Q4.2.1

Draw the following molecules:

*trans*-1,3-dimethylcyclohexane

*trans*-1,2-dibromocyclopentane

*cis*-1,3-dichlorocyclobutane

Solutions

S4.2.1

1

2

3

Contributors

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- Prof. Steven Farmer ([Sonoma State University](#))