Chapter 3. Alkanes and Cycloalkanes

Learning objectives:

1. Name alkanes and cycloalkanes.
2. Write the structures of constitutional (or structural) isomers of alkanes.
3. Draw Newman projections of alkanes in staggered and eclipsed conformations, and arrange the order of stability for these conformations (conformational isomers).
4. Identify cis and trans relationship for the substituents on cycloalkanes.
5. Draw chair conformation of cyclohexane with unambiguous representation of axial and equatorial substituents.
6. Complete the equilibrium of two chair conformational isomers for a substituted cyclohexane, indicate the change for the relative positions of axial and equatorial substituents, and reason the stability between these two isomers.
7. Write the balanced equation for the combustion of alkanes.

* Molecular model kit will be very helpful for learning the material in this chapter.*

Sections to be covered (in the order of delivery):

3.1 Introduction#
3.2 Structure of Alkanes
3.3 Constitutional Isomerism in Alkanes
3.4 Nomenclature of Alkanes
3.5 Cycloalkanes
3.6 The IUPAC system - A general System of Nomenclature
3.7 Conformations of Alkanes and Cycloalkanes*
3.8 Cis - Trans Isomerism in Cycloalkanes*
3.9 Physical Properties of Alkanes and Cycloalkanes
3.10 Reactions of Alkanes
3.11 Sources of Alkanes#

* Sections that will be focused
# Sections that will be skipped

Recommended additional problems

3.12 - 3.42, 3.48 - 3.52
3.2 Structure of Alkanes

(i) Methane

\[
\text{CH}_4
\]

(ii) Ethane

\[
\text{C}_2\text{H}_6
\]

(iii) Butane

\[
\text{C}_4\text{H}_{10} \quad \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3
\]
3.3 Constitutional Isomerism in Alkanes

*Constitutional isomers:* Compounds with the same molecular formula but with different order of attachment (connectivity) of their atoms.

General formula: \( \text{C}_n\text{H}_{2n+2} \)

Examples:

(i) Butane (\( \text{C}_4\text{H}_{10} \))

Normal butane (\( n \)-butane)

\[
\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3
\]

2-Methylpropane or isobutane (\( iso \)-butane or \( i \)-butane)

\[
\text{CH}_3\text{CH}((\text{CH}_3))\text{CH}_3
\]

(ii) Pentane (\( \text{C}_5\text{H}_{12} \))

\[
\begin{align*}
\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 & \quad \text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3 & \quad \text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_3
\end{align*}
\]
3.4 Nomenclature of Alkanes

A. The IUPAC System

*Important to know the prefix for C = 1 to 10 (Table 3.2)*

*Important to know the common alkyl groups (Table 3.3)*

(i) Identify the longest carbon chain.
(ii) Locate the substituent with the lowest number on the parent (main) chain. If equivalent positions are encountered, assign the substituent with higher alphabetical order a higher priority (lower in numbering).
(iii) Place prefix of substituents according to their position on the main chain. Use di-, tri-, tetra-, penta-, hexa- and so on for identical substituents.
(iv) Arrange the substituents, excluding di-, tri-, tetra-, penta-, hexa- and so on, in alphabetical order.

Examples:

(i)

(ii)

(iii)

(iv)

(v)
B. Common Names

Butyl groups ($n$-, iso-, sec-, tert-)

C. Classification of Carbon and Hydrogen Atoms

3.5 Cycloalkanes

General formula: $C_nH_{2n}$
3.6 The IUPAC system - A general System of Nomenclature

**Important infix**

<table>
<thead>
<tr>
<th>Infix</th>
<th>Nature of Carbon-carbon Bonds in the Main Chain</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>-an-</td>
<td>All single (saturated) bond</td>
<td>( \text{H}_3\text{C}-\text{CH}_3 ) Ethane</td>
</tr>
<tr>
<td>-en-</td>
<td>One or more double bonds</td>
<td>( \text{H} \equiv \text{C} \equiv \text{H} ) Ethene (ethylene)</td>
</tr>
<tr>
<td>-yn-</td>
<td>One or more triple bonds</td>
<td>( \text{H} \equiv \text{C} \equiv \text{C} \equiv \text{H} ) Ethyne (acetylene)</td>
</tr>
</tbody>
</table>

**Important suffix**

<table>
<thead>
<tr>
<th>Suffix</th>
<th>Class of Compound</th>
<th>Example</th>
</tr>
</thead>
<tbody>
<tr>
<td>-e</td>
<td>hydrocarbon</td>
<td>( \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 ) Pentane</td>
</tr>
<tr>
<td>-ol</td>
<td>alcohol</td>
<td>( \text{CH}_3\text{CH}_2\text{OH} ) Ethanol</td>
</tr>
<tr>
<td>-al</td>
<td>aldehyde</td>
<td>( \text{H}_3\text{C} \equiv \text{C} = \text{O} ) CH(_3)CHO acetaldehyde</td>
</tr>
<tr>
<td>-one</td>
<td>ketone</td>
<td>( \text{H}_3\text{C} \equiv \text{C} = \text{O} ) \text{CH}_3\text{COCH}_3 ) acetone</td>
</tr>
<tr>
<td>-oic acid</td>
<td>carboxylic acid</td>
<td>( \text{H}_3\text{C} \equiv \text{C} = \text{O} ) \text{OH} \text{CH}_3\text{CO}_2\text{H} ) acetic acid</td>
</tr>
</tbody>
</table>

3.7 Conformations of Alkanes and Cycloalkanes

Conformation: result of single bond rotation

Conformational isomer: same atomic connectivity but different spatial arrangements of atoms.
A. Alkanes

Newman projection:

B. Cycloalkanes

(i) Cyclopentane
(ii) Cyclohexane

Know how to draw chair conformation of cyclohexane.
Know how to show axial and equatorial positions of cyclohexane.
1,3-diaxial interaction (diaxial interaction, axial-axial interaction)
3.8 Cis - Trans Isomerism in Cycloalkanes
3.9  Physical Properties of Alkanes and Cycloalkanes

A. Boiling Points

Boiling points of alkanes increase with increasing molecule weight.

B. Dispersion Forces and Interactions between Alkane Molecules

Dispersion force (van der Waals interaction, electrostatic attraction)
C. Melting Point and Density

Melting points of alkanes are governed by the shape of molecule (packing of molecule) and molecule weight.

D. Constitutional Isomers Have Different Physical Properties

3.10 Reactions of Alkanes

\[ \text{C}_n\text{H}_{2n+2} + \frac{(3n+1)}{2}\text{O}_2 \rightarrow n\text{CO}_2 + (n+1)\text{H}_2\text{O} \]