Nomenclature

IUPAC nomenclature for organic chemistry
What is IUPAC nomenclature?

• A systematic method of naming organic chemical compounds as recommended by the International Union of Pure and Applied Chemistry (IUPAC).
• It provides an unambiguous structure.
• Official IUPAC naming recommendations are not always followed in practice, and the common or trivial name may be used.
rules for alkane nomenclature

• Find and name the longest carbon chain
• Name the groups attached to the longest carbon chain
• Number the chain consecutively, starting at the end nearest a substituted group
• Designate the location of each substituent group
• Assemble the name by listing groups in alphabetical order and the main chain last
# Main chain and alkyl group names

## Main chain names

<table>
<thead>
<tr>
<th>Name</th>
<th># of Carbons</th>
<th>Name</th>
<th># of Carbons</th>
</tr>
</thead>
<tbody>
<tr>
<td>methane</td>
<td>1</td>
<td>hexane</td>
<td>6</td>
</tr>
<tr>
<td>ethane</td>
<td>2</td>
<td>heptane</td>
<td>7</td>
</tr>
<tr>
<td>propane</td>
<td>3</td>
<td>octane</td>
<td>8</td>
</tr>
<tr>
<td>butane</td>
<td>4</td>
<td>nonane</td>
<td>9</td>
</tr>
<tr>
<td>pentane</td>
<td>5</td>
<td>decane</td>
<td>10</td>
</tr>
</tbody>
</table>

## Alkyl group names

<table>
<thead>
<tr>
<th>Name</th>
<th># of Carbons</th>
<th>Name</th>
<th># of Carbons</th>
</tr>
</thead>
<tbody>
<tr>
<td>methyl</td>
<td>1</td>
<td>butyl</td>
<td>4</td>
</tr>
<tr>
<td>ethyl</td>
<td>2</td>
<td>pentyl</td>
<td>5</td>
</tr>
<tr>
<td>propyl</td>
<td>3</td>
<td>Hexyl</td>
<td>6</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Group Name</th>
<th>(CH₃)₂CH—</th>
<th>(CH₃)₂CH₂—</th>
<th>CH₃CH₂CH(CH₃)—</th>
<th>(CH₃)₃C—</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Isopropyl</td>
<td>Isobutyl</td>
<td>sec-Butyl</td>
<td>tert-Butyl</td>
</tr>
</tbody>
</table>
Example

- Longest chain/main chain:
  - 7 carbons (circled)
  - Name: heptane

- Side chain groups:
  - 1-carbon group at position 3
    - Name: 3-methyl
  - 2-carbon group at position 4
    - Name: 4-methyl

Answer:

4-ethyl-3-methylheptane
Naming ring compounds

- Same rules as alkane nomenclature except:
  - A cyclo- prefix is added to the root name
  - Groups are numbered to give multiple substituents the lowest possible numbers
  - When there is only one substituent, it does not need to be numbered
  - A ring can also be named as a substituent
Example

- Answer:
  - 1-ethyl-2-methylcyclohexane

Answer:

cyclopropylcyclopentane
naming alkenes and alkynes

• -Ene suffix for alkene and -yne suffix for alkyne
• The root chain must be the longest chain that includes both carbon atoms of the double bond
• Number the root chain from the end nearest a double bond carbon atom (or triple bond carbon atom)
• The smaller of the two numbers designating the carbon atoms of the double/triple bond is used as the locator of alkenes/alkynes
Examples

- \( \text{CH}_3 \text{CH}_3 \text{CH}_3 \text{CH}_3 \)
- \( \text{H}_3 \text{C} \text{C} \text{H}_3 \text{CH}_3 \text{CH}_3 \text{CH}_3 \)

Answer:
1-cyclobutyl-3-methyl-1-butyne
Naming organic halides

• Same naming rules as before
• Halide substituents are named as fluoro (-F), chloror (-Cl), bromo (-Br), or iodo (-I)

Example:                          Answer:

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

2-chloropropane
Naming Alcohols

• Drop the –ane ending of the parent compound and adding –ol
• When there’s a higher priority group present, -OH can be named as a substituent using the name hydroxy

Example:  

Answer:  3-methyl-1-butanol
Naming Ethers

• Name each of the two carbon groups followed by the word ether (Common naming rule)
• -OR group can also be named as a substituent using the group alkoxy (IUPAC)

Example:

Answer:
cyclopentyl methyl ether or methoxydicyclopentane
Naming aldehydes and ketones

- Aldehydes are named by dropping the -e of the parent name and adding -al
- The substituent name for aldehyde group is formyl
- When one or more -CHO groups are attached to the ring, the ring is named followed by carbaldehyde
- Ketones are named by dropping the -e ending and adding -one
- The substituent name is oxo
Examples

- Answer: \( \text{CH}_3 \text{CH} = \text{C} = \text{H} \)
- 2-methylpropanal

Answer:
3-oxohexanal
Naming Amines

- **Primary Amines (R-NH2):**
  - Replace the –e of the parent group with the word amine
  - Can also name it as a substituent using the name amino

- **Secondary Amines (R2NH):**
  - Use an upper case N to designate the second alkyl group that is on the nitrogen atom

- **Tertiary Amines (R3N):**
  - Named the same way as secondary amines
Examples

• 4-methyl-2-pentamine

• N-methylethanamine

• N-ethyl-N-methylpropanamine
Naming carboxylic acids

- Carboxylic acids are named by dropping the –e ending and adding the –oic acid
- The substituent name for a –COOH group is carboxy

Example: Answer:

2-chlorocyclopentanoic acid
Naming carboxylic acid derivatives

• Acid Halides:
  • Replace the –e ending and add –oyl halide
  • Halide can be bromide, chloride, etc.

• Acid Anhydrides:
  • Symmetrical acid anhydrides are named by replacing acid with anhydride
  • Unsymmetrical acid anhydrides are named by naming each carboxylic acid component and then the word anhydride

• Esters:
  • First name the group that came from the alcohol and drop the –oic acid and add -oate

• Amides:
  • Replace the –oic acid ending with -amide
Examples

- **Answer:**
  - Butanoyl chloride

- **Answer:**
  - Ethanoic propanoic anhydride

- **Answer:**
  - Methyl ethanoate
    (common name: acetate)

- **Answer:**
  - Ethanamide
References

• For more detailed rules and examples including common naming rules, please consult the organic chemistry by wade textbook
• Workshop prepared by Qing Wang