Objectives

After completing this section, you should be able to

1. provide a satisfactory name for an acid halide of given structure.
2. draw the condensed or shorthand structure of an acid halide, given either its commonly used or systematic name.
3. provide a satisfactory name for an acid anhydride of given structure.
4. draw the condensed or shorthand structure of an acid anhydride, given either its trivial or IUPAC name.
5. provide an acceptable name for an amide of given structure.
6. draw the condensed or shorthand structure of an amide, given its trivial or IUPAC name.
7. provide an acceptable name for an ester of given structure.
8. draw the condensed or shorthand structure of an ester, given either its trivial or IUPAC name.
9. provide an acceptable name for a thioester of given structure.
10. draw the condensed or shorthand structure of a thioester, given its trivial or IUPAC name.
11. provide an acceptable name for an acyl phosphate.
12. draw the condensed or shorthand structure of an acyl phosphate, given either its trivial or IUPAC name.

Nomenclature of Acid Halides

The nomenclature of acid halides starts with the name of the corresponding carboxylic acid. The -ic acid ending is removed and replaced with the ending -yl followed by the name of the halogen with an -ide ending. This is true for both common and IUPAC nomenclature. The carbonyl carbon is given the #1 location number. It is not necessary to include the location number in the name because it is assumed that the functional group will be on the end of the parent chain.

Example 21.1.1

[Chemical structures are shown here, one for Propanoyl bromide and another for 2-Methylbutanoyl chloride.]

Propanoyl bromide  2-Methylbutanoyl chloride
(Propionyl bromide)  (2-Methylbutyryl chloride)

The acid anhydride functional group results when two carboxylic acids combine and lose water (anhydride = without water). Symmetrical acid anhydrides are named like carboxylic acids except the ending -acid is replaced with -anhydride. This is true for both the IUPAC and Common nomenclature.

Nomenclature of Anhydrides
Symmetrical anhydrides

A symmetrical anhydride is a carboxylic acid anhydride that has the following general structural formula.

\[
\begin{align*}
\text{O} & \quad \text{O} \\
\text{R}^1 & \quad \text{C} \quad \text{O} \quad \text{C} \quad \text{R}^2
\end{align*}
\]

where \( R^1 = R^2 \) = hydrogen atoms, alkyl groups, aryl groups

Unsymmetrical Anhydrides

A mixed or unsymmetrical anhydride is a carboxylic acid anhydride that has the following general structural formula.

\[
\begin{align*}
\text{O} & \quad \text{O} \\
\text{R}^1 & \quad \text{C} \quad \text{O} \quad \text{C} \quad \text{R}^2
\end{align*}
\]

where \( R^1 \neq R^2 \), but are hydrogen atoms, alkyl groups, aryl groups. When naming unsymmetrical acid anhydrides, name both using alkanoic general method and then put the two names \textit{alphabetically}. Hence, first name each component and alphabetically arranged them followed by spaces and then the word anhydride.
Exercise

Try to name the following compound

Try to draw a structure for the following compound

- 1,2-benzenedicarboxylic anhydride

Common names that you should know

acetic anhydride (Try to name this anhydride by the proper name.)

succinic anhydride (Try to name this anhydride by the proper name.)

Nomenclature of Esters

Esters are made from a carboxylic acid and an alcohol.

Esters are named as if the alkyl chain from the alcohol is a substituent. No number is assigned to this alkyl chain. This is
followed by the name of the parent chain form the carboxylic acid part of the ester with an \( \text{–e} \) remove and replaced with the ending \( \text{–oate} \).

Example 21.1.2

\[
\begin{align*}
\text{Methyl ethanoate} & \quad \text{Ethyl propanoate} \\
H_3C & \quad H_3C \text{CH}_2 \\
\text{C} & \quad \text{C} \\
\text{O} & \quad \text{O} \\
\text{O} & \quad \text{O} \\
\text{CH}_3 & \quad \text{CH}_2\text{CH}_3
\end{align*}
\]

**Nomenclature of Thioesters**

Thioesters are made from a carboxylic acid and an thiol.

\[
\begin{align*}
\text{Ester} & \quad \text{Carboxylic Acid} \\
\text{R} & \quad \text{R} \text{'} \\
\text{C} & \quad \text{C} \\
\text{O} & \quad \text{O} \\
\text{R} & \quad \text{OH} \\
\text{HS} & \quad \text{R} \text{'}
\end{align*}
\]

Thioesters are named as if the alkyl chain from the alcohol is a substituent. No number is assigned to this alkyl chain. This is followed by the name of the parent chain from the carboxylic acid part of the thioester named as an alkane with the ending \( \text{–thiooate} \).

Example 21.1.3

\[
\begin{align*}
\text{Methyl ethanethiooate} & \quad \text{Ethyl propanethiooate} \\
H_3C & \quad H_3C \text{CH}_2 \\
\text{C} & \quad \text{C} \\
\text{O} & \quad \text{S} \\
\text{S} & \quad \text{CH}_3 \\
\text{H}_3C & \quad \text{H}_3C \text{CH}_2 \text{CH}_3
\end{align*}
\]

**Nomenclature of amides**

**Primary amides**

Primary amides are named by changing the name of the acid by dropping the \( \text{-oic acid or -ic acid endings and adding } \text{-amide} \). The carbonyl carbon is given the \#1 location number. It is not necessary to include the location number in the name because it is assumed that the functional group will be on the end of the parent chain.
Secondary amides are named by using an upper case N to designate that the alkyl group is on the nitrogen atom. Alkyl groups attached to the nitrogen are named as substituents. The letter N is used to indicate they are attached to the nitrogen. Tertiary amides are named in the same way.
Exercise

a. Try to draw a structure for N,N-dimethylformamide

b. Try to name the following compound

\[
\text{CH}_3\text{C-}\text{NH}-\text{C-}\text{O}
\]

Name the parent alkane (include the carbon atom of the nitrile as part of the parent) followed with the word -nitrile. The carbon in the nitrile is given the #1 location position. It is not necessary to include the location number in the name because it is assumed that the functional group will be on the end of the parent chain.

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**Naming Phosphates**

**Phosphoryl groups** are derivatives of phosphoric acid, a strong acid that is commonly used in the laboratory. The fully deprotonated conjugate base of phosphoric acid is called a phosphate ion, or inorganic phosphate (often abbreviated 'P\(^i\)'). When two phosphate groups are linked to each other, the linkage is referred to as a 'phosphate anhydride', and the ion is called 'inorganic pyrophosphate' (abbreviation PP\(^i\)).

\[
\begin{align*}
\text{PO}_4^{3-} &\quad \text{phosphoric acid} \\
\text{P}_2\text{O}_{7}^{4-} &\quad \text{inorganic phosphate (P}\(^i\)) \\
\text{P}_4\text{O}_{10}^{8-} &\quad \text{inorganic pyrophosphate (PP}\(^i\))
\end{align*}
\]

When a phosphate ion is attached to a carbon atom on an organic molecule, the chemical linkage is referred to as a phosphate ester, and the whole species is called an organic monophosphate. Glucose-6-phosphate is an example.
If an organic molecule is linked to two or three phosphate groups, the resulting species are called organic diphosphates and organic triphosphates.

Isopententyl diphosphate and adenosine triphosphate (ATP) are good examples:

Oxygen atoms in phosphate groups are referred to either 'bridging' and 'non-bridging', depending on their position. An organic diphosphate has two bridging and five non-bridging oxygens.

When a single phosphate is linked to two organic groups, the term 'phosphate diester' is used. The backbone of DNA is composed of phosphate diesters.
The term 'phosphoryl group' is a general way to refer to all of the phosphate-based groups mentioned in the paragraphs above.

Recall (section 1.4A) that phosphate groups on organic structures are sometimes abbreviated simply as 'P', a convention that we will use throughout this text. For example, glucose-6-phosphate and isopentenyl diphosphate are often depicted as shown below. Notice that the 'P' abbreviation includes the oxygen atoms and negative charges associated with the phosphate groups.

Exercises

Questions

Q21.1.1

Name the following compounds using IUPAC conventions

(a)
Solutions
S21.1.1

a. 3-methylpentanoyl chloride
b. 2-cyclopentylacetamide
c. propyl 2-methylpropanoate
d. cyclohexylbutanoate
e. tert-butyl cyclopentanecarboxylate
f. 1-methylbutylcyclopentane carboxylate
g. N-methyl-3-butenamide
h. (S)-2-hydroxypropanoyl phosphate
i. propyl 2,3-dimethyl-2-butenethioate

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