6.2: NAMING CARBOXYLIC ACIDS AND NITRILES

OBJECTIVES

After completing this section, you should be able to

1. write the IUPAC name of a carboxylic acid, given its Kekulé, condensed or shorthand structure.
2. draw the condensed or shorthand structure of a carboxylic acid, given its IUPAC name.
3. draw the structure of the following carboxylic acids, given their trivial names: formic acid and acetic acid.
4. provide an acceptable name for a nitrile of given structure.
5. draw the condensed or shorthand structure of a nitrile, give either its trivial or IUPAC name.

KEY TERMS

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

- carboxylic acid
- nitrile

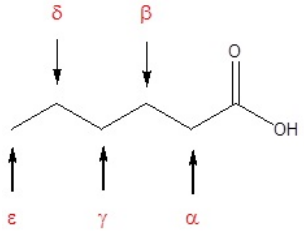
STUDY NOTES

You need not memorize all the trivial names listed in the table, just remember the two names identified in Objective 3, above.

CARBOXYLIC ACIDS, RCO_2H

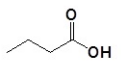
The IUPAC system of nomenclature assigns a characteristic suffix to these classes. The **–e** ending is removed from the name of the parent chain and is replaced **-oic acid**. Since a carboxylic acid group must always lie at the end of a carbon chain, it is always is given the #1 location position in numbering and it is not necessary to include it in the name.

Many carboxylic acids are called by the common names. These names were chosen by chemists to usually describe a source of where the compound is found. In common names of carboxylic acids, carbon atoms near the carboxyl group are often designated by Greek letters. The atom adjacent to the carbonyl function is alpha, the next removed is beta and so on.

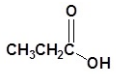


Formula	Common Name	Source	IUPAC Name	Melting Point	Boiling Point
HCO_2H	formic acid	ants (L. formica)	methanoic acid	8.4 ºC	101 ºC
CH_3CO_2H	acetic acid	vinegar (L. acetum)	ethanoic acid	16.6 ºC	118 ºC
$CH_3CH_2CO_2H$	propionic acid	milk (Gk. protus prion)	propanoic acid	-20.8 ºC	141 ºC
$CH_3(CH_2)_2CO_2H$	butyric acid	butter (L. butyrum)	butanoic acid	-5.5 ºC	164 ºC
$CH_3(CH_2)_3CO_2H$	valeric acid	valerian root	pentanoic acid	-34.5 ºC	186 ºC
$CH_3(CH_2)_4CO_2H$	caproic acid	goats (L. caper)	hexanoic acid	-4.0 ºC	205 ºC
$CH_3(CH_2)_5CO_2H$	enanthic acid	vines (Gk. oenanthe)	heptanoic acid	-7.5 ºC	223 ºC
$CH_3(CH_2)_6CO_2H$	caprylic acid	goats (L. caper)	octanoic acid	16.3 ºC	239 ºC
$CH_3(CH_2)_7CO_2H$	pelargonic acid	pelargonium (an herb)	nonanoic acid	12.0 ºC	253 ºC
$CH_3(CH_2)_8CO_2H$	capric acid	goats (L. caper)	decanoic acid	31.0 ºC	219 ºC

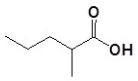
Example (Common Names Are in Red)



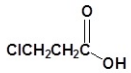
Butanoic acid
(Butyric Acid)



Propanoic acid
(Propionic Acid)



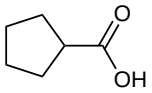
2-Methylpentanoic acid
(β-Methylvaleric acid)



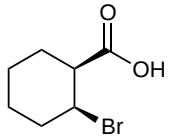
3-Chloropropanoic acid
(γ-Chloropropionic acid)

NAMING CARBOXYL GROUPS ADDED TO A RING

When a carboxyl group is added to a ring, the suffix **-carboxylic acid** is added to the name of the cyclic compound. The ring carbon attached to the carboxyl group is given the #1 location number.

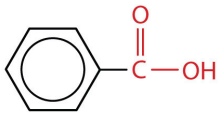


cyclopentanecarboxylic acid



(1S,2S)-2-bromocyclohexanecarboxylic acid

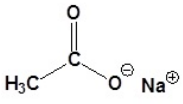
The acid with the carboxyl group attached directly to a benzene ring is called benzoic acid (C_6H_5COOH).



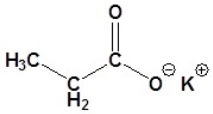
Benzoic acid

NAMING CARBOXYLATES

Salts of carboxylic acids are named by writing the name of the cation followed by the name of the carboxylic acid with the **–ic acid** ending replaced by an **–ate** ending. This is true for both the IUPAC and Common nomenclature systems.



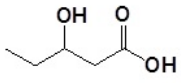
Sodium ethanoate
(Sodium Acetate)



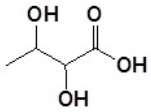
Potassium Propanoate
(Potassium propionate)

NAMING CARBOXYLIC ACIDS WHICH CONTAIN OTHER FUNCTIONAL GROUPS

Carboxylic acids are given the highest nomenclature priority by the IUPAC system. This means that the carboxyl group is given the lowest possible location number and the appropriate nomenclature suffix is included. In the case of molecules containing carboxylic acid and alcohol functional groups, the OH is named as a hydroxyl substituent. However, the **l** in hydroxyl is generally removed.

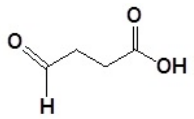


3-Hydroxypentanoic acid

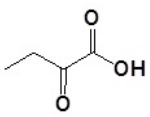


2,3-Dihydroxybutanoic acid

In the case of molecules containing a carboxylic acid and aldehydes and/or ketones functional groups, the carbonyl is named as an "Oxo" substituent.

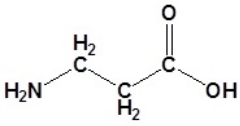


4-Oxobutanoic acid

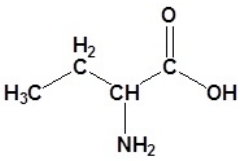


2-Oxobutanoic acid

In the case of molecules containing a carboxylic acid an amine functional group, the amine is named as an "amino" substituent.



3-Aminopropanoic acid

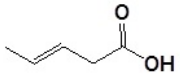


2-Aminobutanoic acid

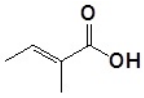
When carboxylic acids are included with an alkene the following order is followed:

(Location number of the alkene)-(Prefix name for the longest carbon chain minus the -ane ending)-(an –enoic acid ending to indicate the presence of an alkene and carboxylic acid)

Remember that the carboxylic acid has priority so it should get the lowest possible location number. Also, remember that *cis/tran* or E/Z nomenclature for the alkene needs to be included if necessary.



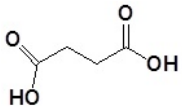
Trans-3-pentenoic acid



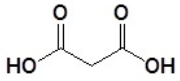
(E)-2-Methyl-2-butenoic acid

NAMING DICARBOXYLIC ACIDS

For dicarboxylic acids the location numbers for both carboxyl groups are omitted because both functional groups are expected to occupy the ends of the parent chain. The ending **–dioic acid** is added to the end of the parent chain name.



Butanedioic acid



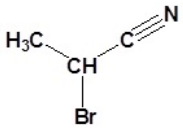
Propanedioic acid

NAMING NITRILES, R−C≡N

A **nitrile** is any organic compound with a −C≡N functional group. In literature the prefix **cyano-** is used interchangeably with the term nitrile to refer to the functional group. Nitriles used to be known as cyanides; the smallest organic nitrile is ethanenitrile, CH_3CN, (old name: methyl cyanide or acetonitrile).

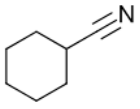
Open chain nitriles are named with the word **-nitrile** after the name of the parent alkane name. Remmber to include the carbon atom of the nitrile as part of the parent chain. For example, CH_3CN has two carbons including the nitrile carbon, therefore it is ethanenitrile. The carbon in the nitrile 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.

Butane nitrile

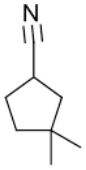


2-Bromopropane nitrile

When a nitrile is the highest priority functional group attached to a cycloalkane, the name of the parent cycloalkane is followed by the word **-carbonitrile**. The ring carbon attached to the nitrile is numbered C1 and the nitrile is not given a number in the name.

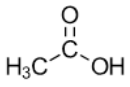


Cyclohexanecarbonitrile

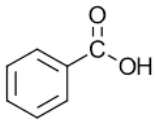


3,3-Dimethylcyclopentanecarbonitrile

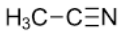
Nitriles are often named based off the common name of the corresponding carboxylic acid. This is done by replacing the -ic acid or -oic acid ending with **-onitrile**. In these cases the nitrile carbon is numbered C1 but the nitrile itself is not given a number in the name.



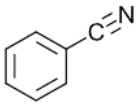
Acetic Acid



Benzoic Acid

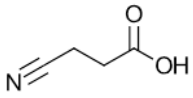


Acetonitrile



Benzonitrile

In the case of molecules containing a carboxylic acid and nitrile functional group, the nitrile is named as a "cyano" substituent. Note! The carbon in the nitrile is not counted as part of the parent chain when named as a cyano substituent.



3-Cyanopropanoic Acid
