2.4: IUPAC Naming of Organic Compounds with Functional Groups

With the ability to identify functional groups, next we will learn how to give IUPAC names to compounds containing a few functional groups, by following a set of rules.

IUPAC NOMENCLATURE of COMPOUNDS with FUNCTIONAL GROUPS

1. Find the longest carbon chain containing the functional group with highest priority (see **Table 2.3**). This chain determines the *parent name* of the compound.
2. Change the ending of the parent alkane/alkene/alkyne to the *suffix* of the highest priority group, which gives the parent name of the compound (usually, drop the last letter "e" before adding the suffix, except for nitrile where the "e" is kept).
3. Number the chain from the end closest to the highest functional group.
4. The other groups are named as substituents by using the appropriate *prefixes*.
5. Assign stereochemistry, E/Z or R/S, as necessary (details in **Chapter 5**).

For naming purposes, the functional groups are assigned with priorities (Table 2.3). If the compound includes more than one functional groups, the one with the ***highest*** priority is the "parent structure" and determines the "parent name"; the other groups will be regarded as "substituents". "Suffix" is used to indicate the name of the parent structure, and "prefix" is for the substituent. The order of the groups listed in **Table 2.3** is based on the *decreasing* order of the priority, where carboxylic acid group is in the highest priority. The groups in the subordinate table have no difference in terms of priority, and they are usually listed in the alphabetic order.

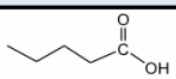
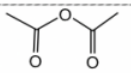
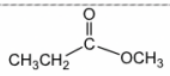
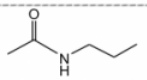
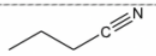
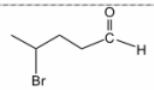
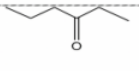
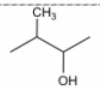
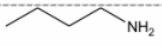
Functional group	Prefix	Suffix	Examples	Name of Example
carboxylic acid	carboxy	–oic acid –carboxylic acid		pentanoic acid
acid anhydride	—	–oic anhydride –carboxylic anhydride		ethanoic anhydride
carboxylic ester	alkoxycarbonyl	–oate –carboxylate		methyl propanoate
amide	amido	–amide –carboxamide		N-propylethanamide
nitrile	cyano	–nitrile (keep "e") –carbonitrile		butanenitrile
aldehyde	oxo	–al –carbaldehyde		4-bromo-pentanal
ketone	oxo	–one		3-hexanone
alcohol	hydroxy	–ol		3-methyl-2-butanol
amine	amino	–amine		butylamine (common name)

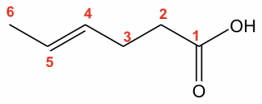
Table 2.3 Naming Priorities of Common Functional Groups

Functional group	Structure	Prefix	Suffix
alkyl halide	R—X (X: F, Br, Cl, I)	halo (fluoro, bromo, chloro, iodo)	—
ether	R—O—R	oxy	ether
sulfide	R—S—R	alkylthio	sulfide
nitro	$-NO_2$	nitro	—
benzene		phenyl	benzene

Table 2.4 Subordinate Groups

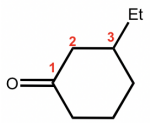
We will go through several examples for more details about the naming rules.

1.



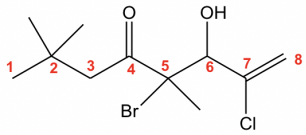
The parent structure is the 6-carbon carboxylic acid with a double bond, so the last name comes from “hexene”. To add the suffix, the last letter “e” will be dropped, so the parent name is “hexeneoicacid”. A number is necessary to indicate the position of the double bond, so the name is “4-hexenoic acid”. The carboxylic acid group is always on the #1 position, so it is NOT necessary to include that number for the position.

2.



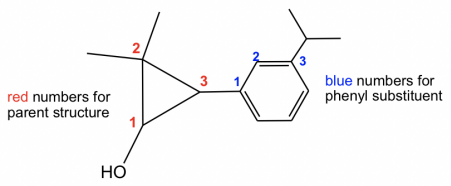
This is a ketone based on a cycloalkane, so the last name comes from “cyclohexane’. By adding the suffix, it become “cyclohexanone”, and the complete name is “3-ethylcyclohexanone”.

3.



With the multiple groups involved, the ketone has the highest priority, so it decides the last name. The 8-carbon alkene chain with ketone should be name as “octenone”. The numbers on the chain should start from the left side to ensure that ketone has the lowest number. When the OH group is regarded as a substituent, it is indicated by the prefix “hydroxy”. So the complete name is “5-bromo-7-chloro-6-hydroxy-2,2,5-trimethyl-7-octen-4-one”.

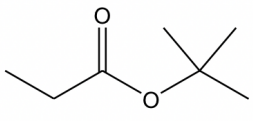
4.



It is not difficult to find the parent structure for this compound, which is a cyclic alcohol, so the last name is “cyclopropanol”. The naming of the substituent with the benzene ring is bit challenging. When benzene is a “substituent”, it is called “phenyl”; and since

there is an isopropyl group on the “phenyl”, the whole substituent is called “3-isopropylphenyl”, and the complete name of the compound is “2,2-dimethyl-3-(3-isopropylphenyl)cyclopropanol”.

5.



In ester, an OR group replaces the OH group of a carboxylic acid. When naming the ester, the name of the R in the OR group is stated first, followed by the name of the acid, with “oic acid” replaced by “oate”. As a net result, the R in the OR is regarded as the “substituent”, even though it is not. So, the complete name of the ester above is “*tert*-butyl propanoate”.

Naming of substituted benzene and benzene derivatives

For substituted benzene, the benzene ring is regarded as the parent structure, and the positions and names of substituents are added to the front.

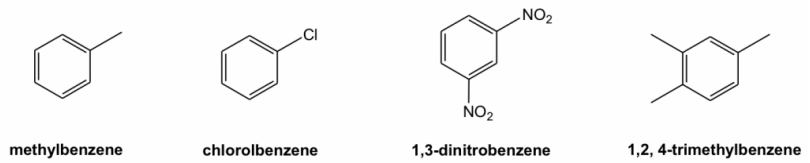
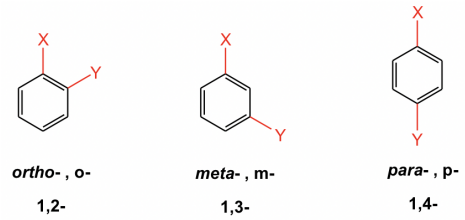


Figure 2.4a Methylbenzene, chlorolbenzene, 1,3-dinitrodenzene, & 1,2,4-trimethylbenzene

For di-substituted benzene, there is another unique way to indicate the relative position of the two substituents by using ortho-, meta- and para-. Although this o-, m-, p- system is the common naming system for benzene derivatives, they have been applied broadly in books and literatures.

- ***ortho*- *(o-):*** 1,2- (next to each other in a benzene ring)
- ***meta*- *(m):*** 1,3- (separated by one carbon in a benzene ring)
- ***para*- *(p):*** 1,4- (across from each other in a benzene ring)



For the following mono-substituted benzene derivatives, phenol, benzoic acid and benzaldehyde, their common names are adopted in the IUPAC system.

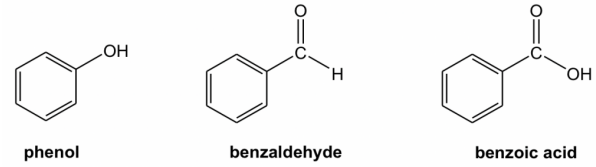
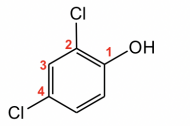


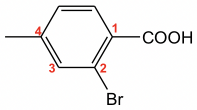
Figure 2.4b Phenol, benzaldehyde, benzoic acid

When other substituents are introduced into those benzene derivatives, the common name will be used as the parent name of the compound with the *base* functional group (OH for phenol, COOH for benzoic acid and CHO for benzaldehyde) given the #1 position. For example:



2,4-dichlorophenol

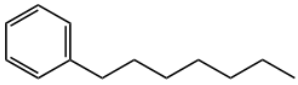
Figure 2.4c 2,4-dichlorophenol



2-bromo-4-methylbenzoic acid

Figure 2.4d 2-bromo-4-methylbenzoic acid

When benzene is connected to a carbon chain that does not contain any higher priority group, benzene is the parent, even if the carbon chain contains more than six carbons. For example, the following compound is heptylbenzene, although the heptyl group has more carbons than benzene.



Heptylbenzene

Figure 2.4e 2-heptanebenzene
