

Nomenclature of some organic compounds

The International Union for Pure and Applied Chemistry (IUPAC) has established rules for organic chemical nomenclature that we will follow in this course. In an IUPAC name, there are four parts:

Prefix–Parent–Infix–Suffix

The **parent** tells how many *carbon* atoms (with a few exceptions to be explained shortly) are in the main chain. The main chain is numbered as explained below.

The **infix** tells the type of carbon–carbon bonding: *-an-* for alkanes, *-en-* for alkenes and *-yn-* for alkynes. If there are both double and triple bonds in the structure, *-en-* comes before *-yn-*. The main chain is numbered so as to give the lowest possible number to the first double bond (if no double bonds, the first triple bond) encountered; this is overridden by the numbering rule for suffixes. The main chain must also have as many functional groups as possible.

The **suffix** tells the family of the molecules, what is the highest-priority non-carbon functionality in the molecule. Several families are given in order of priority in the table above right. The main chain is numbered so as to give the lowest possible number to the functional group controlling the suffix. The main chain must also have as many functional groups as possible.

The **prefix** lists all remaining substituents on the main chain, in alphabetical order. Substituents are numbered so as to give the lowest possible sum of numbers, *provided that this does not conflict with the rules for infixes or suffixes*.

The prefixes *aza-*, *oxa-*, and *thia-* are used as a last resort, when it is easiest to include the heteroatom in the main chain than to name its substituent(s). The heteroatom is then treated as though it substituted for a carbon atom: the heteroatom contributes to the chain length expressed by the parent name.

Family	Description	as Prefix	as Suffix
Alcohol	R–OH	hydroxy-	-ol
Thiol	R–SH	sulfanyl-	-thiol
Amine	R ₃ N	amino-	-amine
Ether	R–O–R	alkoxy-	oxa-
Sulfide	R–S–R	alkylsulfanyl-	thia-
Halide	R–X	halo-	
Hydrocarbon		alkyl-	-e

Some examples

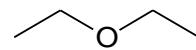
Methyl mercaptan

This compound, commonly added to natural gas so that you can smell leaks, has the structure CH₃SH. Its IUPAC name is methanethiol.

An historical note: Thiols are traditionally called “mercaptans,” and you will sometimes see a “mercapto” prefix for an SH group; this is according to the now-superseded, 1979 IUPAC system of nomenclature.

Diethyl ether

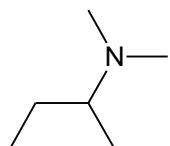
This is the common name of the compound more correctly named “ethoxyethane.” The main chain is ethane (2 carbons); the substituent is an ethoxy group (“ethyl minus “yl” plus “oxy”). The structure of this compound is



N,N-dimethylbutan-2-amine (or -2-butanamine)

The **parent** is “but,” telling us that there are four atoms in the main chain. The **suffix** is “2-amine,” telling us that a nitrogen substituent is attached to atom 2 of the main chain. The **infix** is “an,” telling us that there are no carbon-carbon multiple bonds.

The **prefix** is “N,N-dimethyl.” This means that there are two methyl groups attached to nitrogen, and is the preferred way of naming di- and trialkylamines. The structure of this compound is



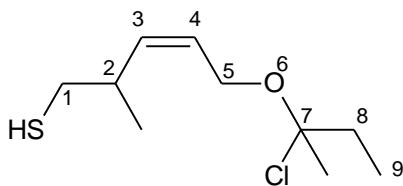
Z-7-Chloro-2,7-dimethyl-6-oxanon-3-en-1-thiol

The **parent** is “non,” telling us that the main chain is 9 atoms long.

The **suffix** is “1-thiol,” telling us that there is a thiol functionality on the first atom in the chain.

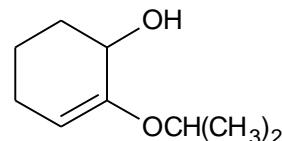
The **infix** is “3-en,” telling us that there is a double bond between atoms 3 and 4 of the main chain. Notice the stereochemical marker “Z”, which tells us the geometry of the double bond.

The **prefixes** are “7-chloro” (a chlorine atom attached to the seventh atom), “2,7-dimethyl” (methyl groups attached the second and seventh atoms) and “6-oxa” (the sixth atom in the main chain is an oxygen). The resulting structure is shown below:

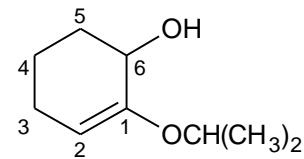


Notice that, while the main chain is nine atoms long, the sixth atom is an oxygen. This is because it is not trivial to name the ether function as an alkoxy group; the ether cannot be named with the “ether” suffix because the thiol takes precedence.

As a further example, consider the structure shown below:



We begin by numbering the ring (which is obviously the main chain). There is a double bond in the ring, and there are two substituents: an OH group, and an isopropoxy group (the isopropyl ether linkage). The alcohol takes priority over the double bond and the ether, so the suffix is “-ol” and the carbon bearing the alcohol is numbered **1**. We number the ring so as to give the lowest possible numbers to the other functional groups:



Since there are six carbons in the ring, the parent name is “cyclohex;” the double bond makes the infix “2-en,” and the isopropoxy group on atom 2 must be named in the prefix. The name is therefore “2-isopropoxycyclohex-2-enol” or sometimes “2-isopropoxy-2-cyclohexenol.”

Why is it unnecessary to specify that the double bond is *E*? that the alcohol is at carbon 1?