I.U.P.A.C. NOMENCLATURE FOR SIMPLE ORGANIC COMPOUNDS

PHILOSOPHY:

Requirements for the name of a chemical compound.

1. a) It must describe the structure completely.
   b) It must not be identical to the name of any other compound.
2. It must be as brief as possible.
3. Preferably, it will be the only name possible.

RULES:

1. Identify the principal functional group (see list in 9).

2. Find the longest continuous carbon chain containing the principal functional group (see 9a) and the greatest possible number of multiple bonds and name it as a hydrocarbon (e.g. "heptane" for 7 carbons, see text for complete list). The chain chosen by this procedure is called the "parent chain." If the parent chain is a ring, the prefix "cyclo" is added to the hydrocarbon name (except "benzene", "toluene", etc.). A parent chain can either be a ring or an open chain but not both. If there is more than one chain of this length, choose:
   a) the chain with the greatest number of double bonds; if that does not decide the issue,
   b) the chain containing the greatest number of substituents; if that does not decide the issue,
   c) the chain which would produce the lowest numbers as described in 4.

3. Identify the substituents and other (not principal) functional groups, assign them prefix names (see 6,9) and place them in alphabetical order. Occasionally substituent names have identical letters but different numbers; the substituent with the lower number on the occasion of the first difference precedes the other.

4. Number the parent chain from one end to the other. This gives each atom of the parent chain a position number. There will be more than one set of numbers possible.
   a) Choose the set which gives the principal functional group the lowest number. If there is more than one of the functional group (e.g. triol) the set of numbers must give the lowest number on the occasion of the first difference in ascending numerical order. If that does not decide,
   b) Choose the set which gives the lowest number to a multiple bond on the first occasion where a difference exists (the first carbon atom of the multiple bond encountered in the chain is its position number). Double bonds have priority over triple. If that does not decide,
   c) Choose the set which gives the lowest number to a substituent position on the occasion of the first difference as you go down the alphabetical list (prepared in 3.); for identical groups, compare the sets of numbers in order.

5. Add to the name of the main chain the suffix(es) indicating the multiple bond(s) and then the principal functional group.
   a) Multiple bonds are indicated by replacing the "ane" ending of the hydrocarbon with "ene" for one double bond, "yne" for one triple bond, "adiene" for two double bonds, "enyne" for one each, etc. In each case the suffix should be preceded by the position number of the multiple bond, e.g. "2,4-diene".
   b) The suffix name for the principal functional group (see 9a) comes after the multiple bond name and is similarly preceded by a position number; if the suffix begins with a vowel, the "e" at the end of the hydrocarbon name is dropped. If there are several of the principal functional group, the multipliers "di", "tri", etc are used, e.g. butane-1,2-diol.

6. Substituents are named in prefixes:
   a) Other functional groups, some of which may not be "principal", are listed in 9a and 9b.
   b) Substituents consisting of carbon chains (with or without other substituents) are named just like a parent chain except:
      i) the carbon atom by which it is attached to the parent chain is always l.
      ii) the "e" is dropped ("ane" if no multiple bonds) and replaced with "yl", e.g. "2,4-dimethylpentyl."
      iii) complex groups are alphabetized under the first letter of their complete name ("d" in "2,4-dimethylpentyl") and are enclosed in parentheses to avoid confusing the numbering systems.
      iv) C_6H_5 is "phenyl"; $C_6H_5CH_2$ is "benzyl". Also allowed are "isopropyl" or "propan-2-yl" for "methylethyl", "isobutyl" for "2-methylpropyl", "*sec*-butyl" or "butan-2-yl" for "1-methylpropyl", "*tert*-butyl" for "dimethylethyl". Since you cannot replicate italics in handwriting, use underline instead.

7. Prefix names are attached to the parent name
   a) in alphabetical order
   b) preceeded by a counting prefix for duplicate substituents: "di", "tri", "tetra", etc. (Strictly, "bis", "tris", "tetrakis" should be used for complex substituents (6b); either is acceptable in this course).
   c) preceded by position numbers, one for each group, separated from the letters of the name by hyphens and from other numbers by commas. Amines and amides may have substituents attached to nitrogen; the position number is then "N".

8. Miscellaneous comments:
   a) Simple amines are usually named by changing "alkan" to "alkyl", e.g. $(CH_3CH_2)_3N$ is triethylamine.
   b) The location of the position numbers in the name can be changed if there is no ambiguity, e.g. hexa-2,4-dien-1-ol can be 2,4-hexadienol-1. Unnecessary numbers may be omitted; e.g. propan-1-oic acid, is propanoic acid.
   c) Another way to prevent confusion of numbering systems (6b) is to prime the numbers on the substituent chain and omit the parentheses.
   d) If you are looking up a particular compound by its name, it is wise to check the system used - some journals put the parent chain first, followed by a comma and

the substituent prefixes. Chemical Abstracts gives each compound an unique code number which can also be used for searches.

e) Recently IUPAC has been working toward meeting requirement 3, having only one name possible, and thus improving computer searching. The numbers now must immediately precede the syllable they locate, as described in 5a) and b). IUAPC has increased flexibility too: substituents may be named using their longest continuous chain as the root and including the point of attachment to the parent chain, e.g. butan-2-yl instead of 1-methylpropyl or *sec*-butyl; there should never be any ambiguity in reading a name like this, and this method is often simpler.

9. a) Common Functional Groups in Order of Decreasing Priority. If there is more than one functional group, the group highest in this priority list becomes the principal functional group and is named in the suffix; the lower priority functional group is named as a substituent in a prefix. You only need to remember the general rule that higher oxidation state has priority over lower, oxygen over nitrogen. Names in parentheses are not required for this course.

Class	**Formula**	**Suffix (Principal)**	**Prefix**
carboxylic acid	- C(=O)-OH	-oic acid[1], or (-carboxylic acid[2])	(carboxy)[2]
ester	- C(=O)-O-R	-yl…-oate[1]	(R-oxycarbonyl)[2]
acid halide	- C(=O)-X	-oyl halide[1]	(haloformyl)[2]
amide	- C(=O)-NH_2	-amide[1]	(carbamoyl)[2]
nitrile	-C≡N	-nitrile[1]	cyano-[2]
aldehyde	- C(=O)-H	-al[1]	(oxo)[1]
ketone	- C(=O)-	-one[1]	(oxo)[1]
alcohol	-O-H	-ol	hydroxy-
amine	-NH_2	-amine	amino-

[1]The carbon atom shown is not part of this name; it must be counted in the parent chain e.g. $CH_3CH_2CO_2H$ propanoic acid.

[2]The carbon atom shown is part of this name and is not counted in the parent chain.

b) Other "functional groups" which are never considered principal functional groups

Class	Formula	Suffix	Prefix (substituent)
ether	-O-R	NA	R-oxy- (e.g. ethoxy-)
halocarbons	F,Cl, Br,I	NA	halo- (e.g. fluoro-)
azide	$-N=N^+=N^-$	NA	azido-
nitro	$-NO_2$	NA	nitro-

9. Double Check

a) Each functional group, multiple bond and substituent must have a number; e.g. if you have "trimethyl", it must be preceded by three position numbers, e.g. "2,2,5-".
b) Have you accounted for every atom in the molecule? An atom may be mentioned in the parent chain, suffix(es) or prefix(es). Have you counted any more than once?
c) A parent chain may not include both cyclic and non-cyclic components.
d) When in doubt, cover the structure and try to draw it from your proposed name -- be honest!

References:

IUPAC Nomenclature of Organic Chemistry, Sections A,B,C,D,E,F and H, 1979 Edition; Pergamon Press, New York 1979.
Homer A. Smith, Jr. *J. Chem. Educ.* **1992**, *69*, 863 - 865.

IUPAC.97: LMS 79, 87, 89, 90, 91, 93, 97