

IUPAC NOMENCLATURE OF HYDROCARBONS

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. Find the longest carbon chain which contains the greatest number of double or triple bonds, and name it as a hydrocarbon (e.g. "heptane" for 7 carbons; see text for complete list). This chain is the parent chain. If the longest chain is a ring, the prefix "cyclo" is added to the hydrocarbon name (except "benzene", "toluene", etc.). The parent chain may be either a ring or an open chain *but not both*. If there is more than one chain of this length, choose the chain containing the greatest number of substituents. If there is still more than one chain possible, choose the one with the lowest numbers (as determined in 3).
2. Identify the substituents; assign them prefix names (see 5) and place them in alphabetical order. (Occasionally substituents have identical word names but different numbers; the substituent with the lower number on the occasion of the first difference precedes the other alphabetically.)
3. Number the parent chain from one end to the other; this gives each substituent a position number. There will be more than one set of numbers possible.
 - a) 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,
 - b) 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 2; for identical groups, compare the sets of numbers in order.
4. Add to the name of the parent chain the suffix(es) indicating the multiple bond(s). 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, "ynene" for one each, etc. In each case the suffix should be preceded by the position number (see 6b) of the multiple bond, e.g. "2,4-diene".
5. Substituents are named in prefixes. Substituents consisting of carbon chains (with or without other substituents) are named just like the parent except:

- a) The carbon atom by which it is attached to the parent chain is always 1.
 - b) The "e" is dropped ("ane" if no multiple bonds) and replaced with "yl", e.g. "2,4-dimethylpentyl."
 - c) Complex substituents 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.
 - d) C₆H₅ is "phenyl"; C₆H₅CH₂ 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.
6. Prefix names are attached to the parent name
- a) in alphabetical order,
 - b) preceded by a counting prefix for duplicate substituents: "di", "tri", "tetra", etc., which is
 - c) preceded by position numbers, one for each group, separated from the letters of the name by hyphens and from other numbers by commas.
7. Double Check.
- a) Each multiple bond and substituent must have a number; e.g. if you have "trimethyl", it must be preceded by three numbers, e.g. "2,3,5-".
 - b) Have you accounted for every atom in the molecule? An atom may be mentioned in the parent chain, suffix or prefix(es), but may only be mentioned *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.