Some Rules for Organic Nomenclature for Chem 111 (vs. 2019 for 2020)

These rules allow you to go from structure to name for relatively simple molecules, and show how condensed structures are written. ChemDraw or similar software is useful for naming complex molecules – for instance, those with multiple functional groups.

A. Alkanes, Haloalkanes and Nitroalkanes. Use the following rules:

(1) Find the main (longest continuous) carbon chain. The root name gives the # of carbons: meth, eth, prop, but, pent, hex, hept, oct, non, dec, undec, dodec, tridec, tetradec, etc., and is followed by the “ane” suffix for alkanes.

(2) If there is a tie for longest chain, choose chain with most substituents. If still a tie, use rule 3.

(3) Number in direction to give lowest number to first (or if tie, second, etc.) substituent. If still tied, use the chain/direction that puts substituents earlier in alphabetical order at the lowest numbered position.

(4) Duplicate substituents of the same kind get enumerative prefixes: di-, tri-, tetra-, penta-, hexa-, etc.

(5) Substituents occur within name in alphabetical order, ignoring italicized isomer prefixes (iso is not italicized) and also ignoring enumerative prefixes: bromo-, butyl- (CH₂CH₂CH₂CH₂ or C₄H₉), sec-butyl- (CH(CH₃)CH₂CH₂ or s-C₄H₉), tert-butyl (C(CH₃)₃ or t-C₄H₉), chloro-, ethyl- (CH₂CH₃ or C₂H₅), fluoro-, iodo-, isobutyl- (CH₂CH(CH₃)₂ or i-C₄H₉), isopropyl- (CH(CH₃)₂ or i-C₃H₇), methyl (CH₃), nitro (NO₂), propyl- (CH₂CH₂CH₂ or C₃H₇).

(6) Use dashes before and after substituent numbers and end with main chain name: for instance: 5,6-dichloro-4-isobutyl-3,3-dimethyloctane. See skeletal structure at right; the condensed structure is CH₂CH₂C(CH₃)₂CH(i-C₄H₉)CH(CH₂CH₂CH₂)CH₃.

B. Cycloalkanes: The suffix is still “ane”; “cyclo” is added before the root name. If two rings are connected by one bond, the larger ring gives the base name. Rule 3 is used to choose position 1 and whether numbering will be clockwise or counterclockwise around ring. 2-ethyl-6-isopropyl-1,1-dimethylcyclohexane.

C. Ethers: Substituents on benzene are numbered as for cycloalkanes. A C₆H₅ aromatic substituent is “phenyl”.

D. Alkenes and alkynes: Allyl (-CH₂CHCH₂) and vinyl (-CHCH₂) are alkene substituents that can be present, for instance, on cycloalkanes. The lower number of the two multiply-bonded carbons is used before the –ene or –yne suffixes (4-methylpent-2-ene = CH₃CHCHCH(CH₃)₂), or optionally before the root name (4-methyl-2-pentene). Dienes and enynes are possible: hexa-2,4-diene (CH₂CHCHCHCH₂CH₃) or hex-1-en-4-yne (CH₂CHCH₂CCH₃). In acyclic alkenes and alkynes, the main chain is chosen (if possible) to include all double and/or triple bonds (overrides rule #A1), and is numbered in the direction that results in the lowest numbered multiple bond (overrides rule #A3; the positions of substituents are used only as a tie-breaker).

E. Amines: Use –amine as a suffix and numbering to indicate its position (if needed). If the amine is secondary or tertiary, use “N–” to indicate the smaller substituents on the nitrogen. For instance: N,N-dimethylbutan-1-amine = CH₃CH₂CH₂CH₂N(CH₃)₂. By rule P, an alternative name for this compound is butyl dimethyl amine.

If another functional group with higher priority (i.e. those listed below) is present, -NH₂ is treated as a substituent named “amino”.

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F. Amines: Use –amine as a suffix and numbering to indicate its position (if needed). If the amine is secondary or tertiary, use “N–” to indicate the smaller substituents on the nitrogen. For instance: N,N-dimethylbutan-1-amine = CH₃CH₂CH₂CH₂N(CH₃)₂. By rule P, an alternative name for this compound is butyl dimethyl amine.

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For instance: 4-ethyl-2-methylhexane = (CH₃)₂CHCH[(OC₃H₇)₂C₆H₅]C₂H₅. See rule P for alt. naming.
G. **Alcohols & Thiols:** Use –ol or -thiol suffix, and choose main chain to include the carbon attached to the –OH/SH. Number in the direction to give the –OH the lowest number. *Officially*, the number is placed just before –ol (i.e. CH₂CHOHCH₂CH₃ is butan-2-ol), but many chemists write and say “2-butanol”. This is a.k.a. sec-butyl alcohol; see rule P.

*If another functional group with higher priority (i.e. those listed below) is present, -OH and -SH are treated as substituents named “hydroxy” and ‘mercaptop”, respectively.*

H. **Ketones:** Use the –one suffix, along with a number to indicate which number of the chain is the carbonyl carbon. For example, pentan-2-one (or the easier to say 2-pentanone) = CH₃COCH₂CH₂CH₃. See rule P for alternative naming.

I. **Aldehydes:** Use –al suffix. The -C(=O)H aldehyde is always considered to be carbon 1 of the chain. For example, 5,5-dimethylhexanal is (CH₃)₃CCH₂CH₂CH₂CHO (aldehyde condensed structures *end* with position 1).

J. **Nitrile:** Use -anenitrile suffix. The nitrile carbon is C-1. 4-iodobutanenitrile = CH₂ICH₂CH₂CN.

K. **Amide:** R-C(=O)-NR'R'' is named with –amide as suffix. The R’ and R” substituents are added to the name with “N-“ in place of a numbered substituent marker. N,N-dimethylbutanamide has R=C₃H₇ and R’ = R” = CH₃.

L. **Acid halide:** Use “–oyl [halide]” as suffix; C-1 is carbonyl carbon. Propanoyl chloride = CH₃CH₂COCl.

M. **Esters:** R-C(=O)-OR’ is named as if R’ is a substituent added to the deprotonated anion (of carboxylic acid) that forms if R’(+) were removed. Two words with space between: ethyl butanoate is CH₃CH₂COOCH₂CH₃.

N. **Sulfonic acids:** Use “-sulfonic acid” as a suffix. Propane-1-sulfonic acid = CH₃CH₂CH₂SO₃H.

O. **Carboxylic Acids:** Use “–oic acid” as a suffix (or “-oate” if the acid has lost H⁺ to form an anion). The carbonyl carbon is C-1 and usually *ends* the condensed structure: 3-chloropropanoic acid is CH₂ClCH₂COOH.

P. **Alternative multi-word names for alcohols, ethers, ketones, amines & (mono)haloalkanes:** The last word is “alcohol” (1), “ether” (2), “ketone” (2), “amine” (1, 2 or 3) or halide name (“chloride”, etc.; 1). The number in parentheses is the number of substituents (ROH, ROR’, RCOR’, RN(R')R”, RX) that must be specified. Substituents each get their own word ending in –yl and separated by spaces. For instance: ethyl phenyl ketone. With two or three identical substituents, use enumerative prefixes: i.e. diethyl ether or triethyl amine.

Q. **Special names in wide use by chemists:**

1 carbon: formaldehyde, formic acid, formate, formamide.

2 carbons: acetic acid, acetate, acetaldehyde, acetamide, acetyl chloride, acetonitrile (but acetone is CH₃COCH₃ = 3 carbons).

3 carbons: propionic acid, propionaldehyde, etc.

6 carbons (phenyl + OH or NH₂): phenol, aniline.

7 carbons (phenyl + 1 C): toluene (=methylbenzene), benzaldehyde, benzoic acid, benzoate, benzamide, benzyl alcohol, benzyl amine, benzonitrile.

R. **When to use “1-“:** Use “1-“ if *and only if needed* to avoid ambiguity. (i.e. “propan-1-ol”, but not “ethan-1-ol” and not “1-chlorobenzene”). Don’t use “1-“ for aldehydes, acids, amides, etc. where C-1 is always in the functional group.