Advanced IUPAC Nomenclature XIII

Multiple Functional Groups

- **Priority of functional groups in descending order:**
  - Carboxylic Acids
  - Carboxylic Acid Derivatives (Class I carbonyls)
    - Anhydrides
    - Esters
    - Acid halides
    - Amides
    - Nitriles
  - Aldehydes and Ketones (Class II carbonyls)
    - Aldehydes
    - Ketones
  - Alcohols
  - Thiols
  - Amines
  - Pi bonds
    - Benzene
    - Alkenes
    - Alkynes
  - Alkanes / Ethers / Haloalkanes

- **Endings for functional groups**
  - Carboxylic Acids: drop the last –e from the base name, add –oic acid.
    - propanoic acid = CH_3CH_2COOH
    - A single carbon on a ring adds -carboxylic acid to the full alkane name.
  - Anhydrides: drop the acid from the name(s) of the acid portions and add anhydride.
    - $CH_3CH_2COOCOCH_3$ ethanoic propanoic anhydride
  - Esters: drop the last –e from the base name, add –oate. The OR' portion is named as a separate alkyl group in front.
    - Methyl 2-methylpropanoate = $(CH_3)_2CHCOOCH_3$
    - A single carbon on a ring adds –carboxylate to the full alkane name.
    - Cyclic esters are lactones or oxa-2-cycloalkanones.
  - Acid Halides: drop the last –e from the base name, add –oyl halide.
    - But-2-enoyl chloride = $CH_3CH=CHCOCl$
    - A single carbon on a ring adds –carbonoyl halide to the full alkane name.
  - Amides: drop the last –e from the base name, add –amide. Substituents on the nitrogen are N-alkyl substituents.

        - N-ethylpentanamide = $CH_3CH_2CH_2CH_2CONHCH_2CH_3$
        - A single carbon on a ring adds –carboxamide to the full alkane name.
        - Cyclic amides are lactams or aza-2-cycloalkanones
    - Nitriles: add –nitrile to the end of the alkane name.
        - 2-bromo-4,4-dimethylpentanenitrile = $(CH_3)_3CCH_2CHBrCN$
        - A single carbon on a ring adds –carbonitrile to the full alkane name.
    - Aldehydes: drop the last –e from the base name, add –al
        - 3-methylhept-6-ynal = $HCCCH_2CH_2CH(CH_3)CH_2CHO$
        - A single carbon on a ring adds –carbaldehyde to the full alkane name.
    - Ketones: drop the last –e from the base name, add –one
        - Hex-5-en-2-one = $CH_3COCH_2CH_2CHCH_2$
    - Alcohols: drop the last –e from the base name, add –ol
        - 3-methyl-2-pentanol = $CH_3CHOHCH(CH_3)CH_2CH_3$
    - Amines: drop the last –e from the base name, add –amine
        - *N*-ethylpent-4-en-1-amine = $CH_3CH_2NHCH_2CH_2CH_2CHCH_2$
        - The longest chain is the base name, other alkyl groups on the N are named as *N*-alkyl substituents
    - Alkenes: drop the last –ane from the base name, add –ene
        - 1-butene = $CH_2CHCH_2CH_3$
        - The –en ending remains even when other functional groups are present
    - Alkynes: drop the last –ane from the base name, add –yne
        - 1-pentyne = $HCCCH_2CH_2CH_3$
        - The –en ending remains even when other functional groups are present
        - Compounds with alkenes and alkynes are –enynes
    - Ethers: No ending change named as alkoxyalkanes
        - $CH_3CH_2OCH_2CH_2CH_3$ = 1-ethoxypropane

- **Notes:**
    - Many functional groups can have multiples and will use the same prefixes as any other substutiuent. E.g., 1,4-butanediol or 1,5-pentanedioic acid. The terminal –e is then left for ease of pronunciation.

- **References:**

- http://en.wikipedia.org/wiki/IUPAC_organic_nomenclature (Less technical)
- http://www.acdlabs.com/iupac/nomenclature/ (More detailed, more technical)
- Organic Chemistry: Structure and Function 5th Ed., Vollhardt, K. P. C., Schore, N. E., W. H. Freeman and Co., New York, 2007

IUPAC Nomenclature of organic compounds with multiple functional groups

1) Find the longest chain of continuous carbons that includes **the highest priority functional group.** This is now the main chain. Name this chain as if it were a straight chain alkane.
2) Use the functional group suffix for the highest priority functional group.
    a. Alkenes and alkynes will still get endings even if they are not the highest priority group (e.g., an alkene with an alcohol in the same compound would have the ending –enol)
3) Count the carbons in the main chain left to right and right to left. The direction you *first* run into the high priority functional group is the direction use to number the chain. Lower priority substituents no longer matter only the highest priority substituent.
    a. If the numbers are the same go to the next highest priority group.
    b. If the numbers are the same for all functional groups use alphabetical order.
4) Give each substituent a number according to which carbon it's attached to.
    a. Numbers for alkenes and alkynes correspond to the lower numbered of the two carbons in the bond.
    b. Substituents on a nitrogen are *N*-alkyl substituents
5) List the substituents in alphabetical order in front of the main chain as you would in an alkane.
    a. Lower priority functional groups are listed as their substituent name.
    b. Alkenes and alkynes remain in the ending and are never listed in front of the main name.
6) Multiple substituents of the same kind are combined and given a prefix to indicate the number, (di-, tri-, tetra-) these prefixes do not count towards alphabetical order unless they are part of a branched chain.
7) List any relevant stereochemistry in front of the substituents. Including *cis- / trans-* or *E / Z* of the alkenes and *R / S* of chiral carbons. Stereochemistry is always italicized and if multiple stereocenters are present the position of the stereochemistry is indicated (e.g. *2R,3S,4R)*.