Organic Structure and Nomenclature – Alkanes

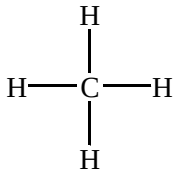
Last semester, you learned the systematic method used to name simple inorganic molecules. NMR is a technique that is highly valuable for determining the structure of organic molecules and, so, we must be able to name and draw structures of those molecules for this technique to be valuable. We'll begin by doing a little bit of review from CHM 211, followed by learning to draw molecules the way organic chemists do, and finally how to name those molecules.

Review and Molecular Structure

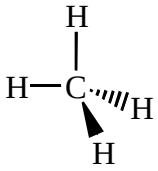
Organic compounds all share the feature that they contain both carbon and hydrogen atoms, indeed the vast majority of compounds containing carbon are organic and from here forward you should assume that all of the compounds we discuss are organic unless you're told otherwise.

Carbon will nearly always form 4 bonds in organic molecules. This can come in the form of 4 single bonds (tetrahedral), 2 single bonds and a double bond (trigonal planar), a triple bond and single bond (linear), or, very rarely, 2 double bonds (linear). The shapes around the carbon atoms follow the corresponding VSEPR shapes you learned in Chapter 9. You should go back and review these shapes now. There are also webpages ("Molecular Graphics") linked from the course website that provides a visualization of many of the molecules that you will encounter in this course.

To begin a discussion of how these molecules are represented on paper, we'll use examples. Methane, CH_4, consists of a carbon atom bound to 4 hydrogen atoms arranged about a tetrahedron. The simple stick structure you saw in CHM 211 would depict methane as



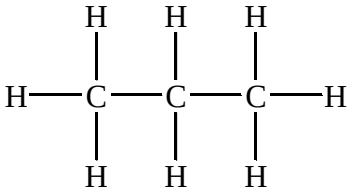
Unfortunately, this picture suggests that methane is square, while it is tetrahedral. For this reason we frequently draw methane like this.

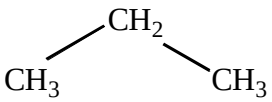


The solid triangle tells you the hydrogen is coming out of the paper towards you, while the dashed line means that it lies behind the plane of the paper.

Likewise the 3 carbon alkane, propane, can be written out a number of ways:

C_3H_8 $CH_3CH_2CH_3$





The last 3 pictures have the advantage of showing atom connectivity, but clearly if each carbon is tetrahedral, the molecule isn't going to have a linear carbon backbone and the final picture has the advantage of showing this as well. We'll make considerable use of this type of drawing in this course.

Alkane Nomenclature

Alkanes are molecules that contain only carbon and hydrogen and have the carbons attached to one another by only single bonds. The only exception is methane, which has only one carbon. Alkanes can all be named systematically. The following rules describe how:

1) All alkanes end in "–ane."
2) Pick out the longest continuous chain of carbon atoms in the molecule. Anything attached to that chain, including other hydrocarbon groups, is a substituent group. The alkane chain is named according to the following sequence:

   1 C = methane 3 C = propane

   2 C = ethane 4 C = butane

   all other compounds use Greek prefixes to indicated chain length

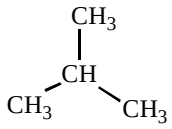
   5 C = pentane 8 C = octane

   6 C = hexane 9 C = nonane

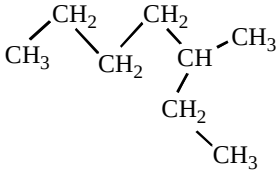
   7 C = heptane 10 C = decane

3) If the alkane has substituents, begin numbering by choosing the side of the alkane with a substituent closest to the end. Do not use numbers if they are not needed. For example, methylpropane does not need to have a "2-" in front (i.e. 2-methylpropane), because the only place you can put the substituent is on the middle carbon. (What do you call the molecule if the methyl group is placed on the first carbon?)
4) Hydrocarbon substituents begin with the same letters as the chains, but end in "–yl." (e.g. CH_3– = methyl).
5) If there is more than one group attached, list them in alphabetical order.
6) When two *identical* numbering schemes exist, the substituent coming first alphabetically should be assigned the lower number.
7) With cycloalkanes, no number is needed if there is only one substituent. If there are two or more substituents bound to the ring, the one which comes first alphabetically is assigned the lower number.

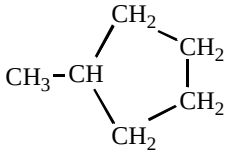
Some examples of how to name alkanes appear below.



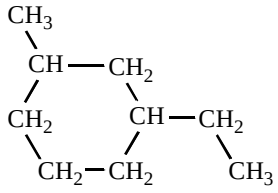
methylpropane



3-methylheptane

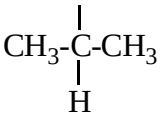


methylcyclopentane

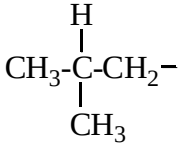


1-ethyl-3-methylcyclohexane

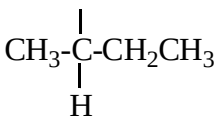
There are also some common (or 'trivial') names used for organic chemicals. One type is the old systematic method. Chemists frequently use these names and you'll encounter them occasionally in this course. For example, the methylpropane used as an example is called isobutane under the old system. The most important saturated hydrocarbon side chains with common names are:



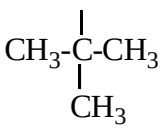
isopropyl



isobutyl



sec-butyl



tert-butyl

In general, the prefix "iso" yields a group with the formula $(CH_3)_2CH(CH_2)_n$-, where n is a positive integer. Thus, isopropyl has n = 0 and isobutyl has n = 1. We'll encounter the other type, unique names, in later sections.

The carbon atoms presented so far may be classified several different ways. An important designation system with respect to NMR identifies the number of hydrogen atoms bound to a carbon. Carbon atoms with 3 hydrogens bound are necessarily methyl (groups). Those with two hydrogen atoms are called methylene groups, while those with only one bound hydrogen are called methines (rarely methynes). Carbons without any bound hydrogen atoms are quaternary carbons.

Finally, there is the existence of isomers. These are compounds with the same formula, but a different arrangement of the atoms. For example, butane and methylpropane both have the formula C_4H_{10}, but in the former molecule there are 4 carbons attached in a chain, while in the latter case, there are 3 carbons bound to a central carbon atom. Nearly all organic compounds with more than 4 carbon atoms have at least one isomer, with the number of isomers per formula increasing with increasing numbers of carbon atoms.