3. THE LANGUAGE OF ORGANIC CHEMISTRY: How we draw organic compounds and how we name them.

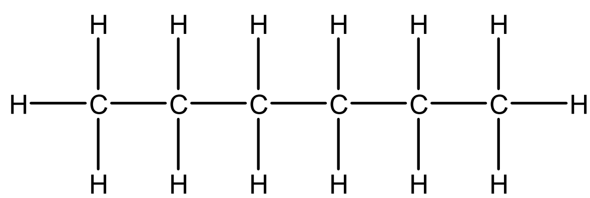
In order for us to have meaningful conversations about organic chemistry, we need a common language. We need to know how to draw molecules that we really can't see and we have to know how to verbalize those pictures. So, the first thing we need to do is to learn how to draw organic molecules and then, give them names. We need to learn how to "speak" organic chemistry.

3.1. Rings and Chains

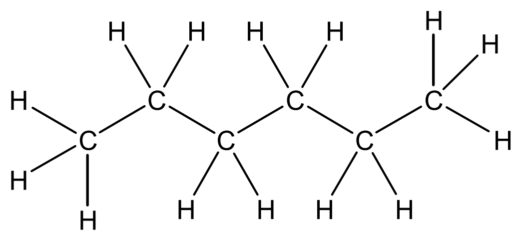
The two most important elements in organic chemistry are C and H. While we will also play with N, S, O, Cl, Br, and I quite a bit, we first have to deal with C and H. Compounds containing only C and H form the most fundamental class of organic compounds, ***hydrocarbons*** (we'll talk more about their chemistry later…). There are two basic structural forms you need to know…rings and chains.

chain = "linear" arrangement of C atoms to form an organic molecule
ring = cyclic arrangement of C atoms to form an organic molecule.

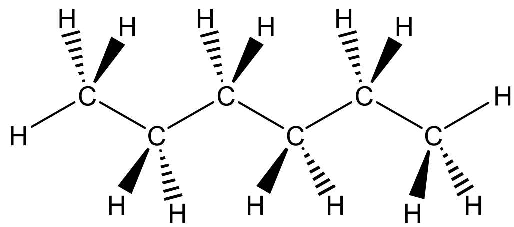
Lets draw chains first. So, lets draw a straight-chain molecule with the formula C_6H_{14}. At first you might draw something like this…



…a perfectly good Lewis structure. The above compound is called hexane, and is a saturated hydrocarbon. This representation makes it seem like the C's are all in a nice straight row. Nothing could be farther from the truth. If you recall, carbon likes to have 4 bonds around it due to hybridization (more on that later). The sp^3 carbon has a tetrahedral geometry. That means that the C's should be in a kind of zigzag…

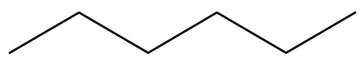


Now, this is better, but our hexane molecule looks flat. Is pentane flat? No, it exists in 3-D. So, we need to show the 3-D nature of the molecule. How do we do that? To do this we use WEDGES and DASHES. A wedge designates something as coming out of the plane of the page. A dash, designates something as receding behind the plane of the page. Normal lines connect all things that are in the same plane as the page. So, a more accurate picture would be…



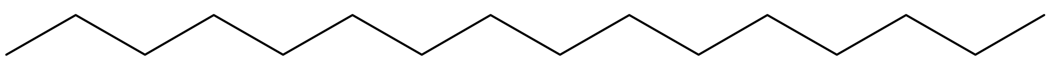
This is better! We have a good 3-D structure. But, can you imagine the time spent drawing everything like this? Ugh…we'ld all get writers cramp. So, a shortcut is needed.

Now, the first, unwritten rule of drawing organic molecules is that you only draw what you need to see (i.e., what is important). For hexane, do we really need to see all the hydrogens? Or can we just know that they are there? Do we really need to show the 3-D nature all the time? I (and countless others) vote "NOT" and thus prefer to draw the following…



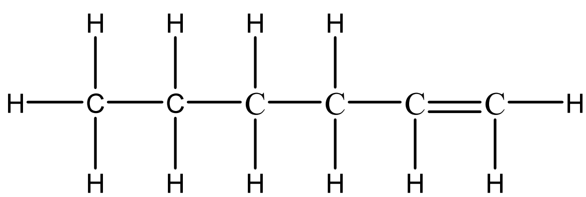
In this ***line structure***, each line represents a C-C bond. Each joint is a carbon. Each end of a line is a carbon. You see four joints and 2 ends…that equals 6 carbons. The hydrogens are implied. The zig-zag denotes the sp^3 nature of the C-C bonds. The above is therefore the preferred representation of the hydrocarbon "hexane" in a chain configuration.

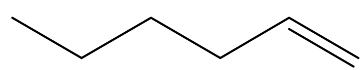
You draw all other chains the same way. How about $CH_3(CH_2)_{14}CH_3$ ($C_{16}H_{34}$, hexadecane)? No sweat…



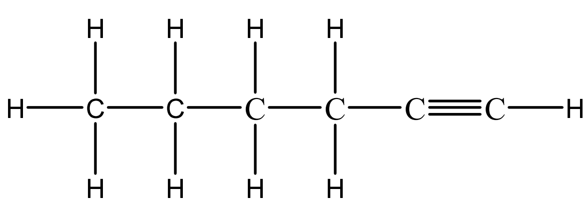
…easy.

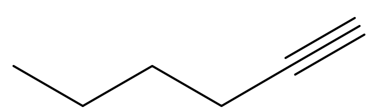
What if you want to draw a C-C double bond? Well, if one line equals one bond, then surely 2 lines equals a double bond. How about this for hexene (hexane with a double bond)…





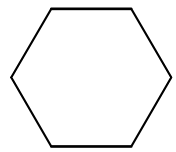
Triple bonds? Yup, three lines.



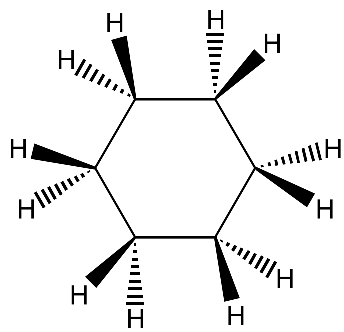


hexyne

So, how about rings? ***For now*** we will draw all rings as flat entities. That will change later, but for now, if we want to draw the ring form of hexane (C_6H_{12}), we would draw a hexagon…



Remember, each kink is a carbon and the hydrogens are there, but we choose not to show them (they are implied). If we really want to show the 3-D nature of the hydrogens we can augment our ring with wedges and dashes…



Again, the wedges are indicate something coming out of the plane of the page, the dashes indicate something going back behind the plane of the page and the lines are IN the plane of the page.

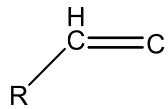
Ok, so, chains and rings are the backbones of organic chemistry… But what about the other elements? You know, the FUNCTIONAL GROUPS?

3.2 Functional Groups

Before you learn how the pieces of a puzzle fit together, you have to be aware of the pieces. In organic chemistry, those pieces are called functional groups. So, what are these? A functional group is a collection of atoms that make up small molecular units within a larger molecule that have reasonably distinct and predictable chemical properties and reactivity. You must be able to recognize them on sight, else you will be hopelessly lost.

In this first semester we are going to deal primarily with hydrocarbons and their simple transformations into compounds which contain some of the functional groups below. We will deal with the specific chemistry unique to each group and family of compounds in due time…but not today. The important groups we will encounter this semester include…

alkyl $R-CH_3$

alkene


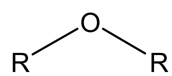
alkyne $R-C\equiv CH$

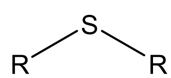
halogens -F, -Cl, -Br, -I

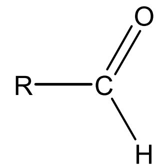
alcohol $R-OH$

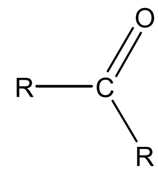
thiol $R-SH$

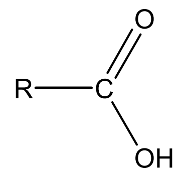
amine $R-NH_3$

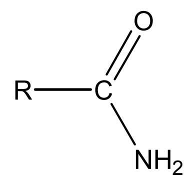
ether


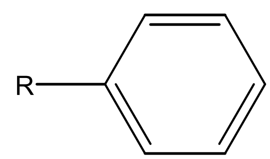
sulfide


aldehyde


ketone


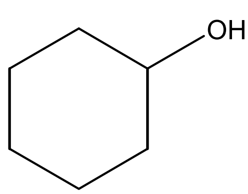
acid


amide


phenyl


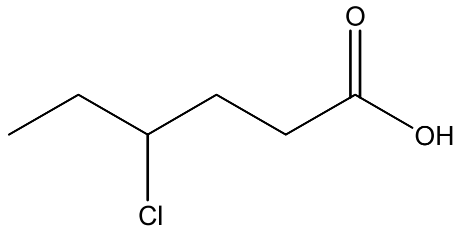
The "R" represents a generic "alkyl" group. R can be hexane or cyclohexane, or any other assemblage of C and H to form a hydrocarbon you can dream up. However, in most of the examples (all in fact, I think) R actually means either "R-CH_2-", such that there is either always a -CH_2- (methylene) group attached to the functional group, or "CH_3-", a methyl group.

For example, lets take our cyclohexane ring and put an alcohol group on it. No problem…



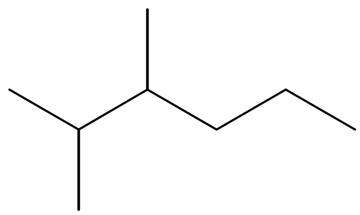
cyclohexanol

How about taking the hexane chain and adding an acid and a chlorine? Again, no sweat…



4-chlorohexanoic acid

How about if we take the hexane chain and add another more R groups to it? Say, two methyl (CH_3-) groups?



2,3-dimethylhexane

The above is called a BRANCHED compound. It consists of a chain with, well, branches. Like a tree. The branches are normally other R groups.

So, how many different compounds can you make up and draw given what little you have seen so far? More than you can count. Trust me.

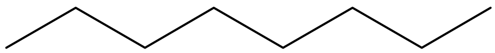
3.3 IUPAC: How we name organic compounds

So, we can draw structures…but what do we call them? I put names next to some compounds, but why did I call them that? To name organic compounds, we turn to **IUPAC** rules (International Union of Pure and Applied Chemistry…check out the CRC handbook).

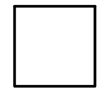
The naming of organic compounds is, first and foremost, based on the consideration that all compounds are derivatives of the longest single continuous carbon chain in the compound. Therefore you have to know the names for each chain length. The "ane" ending is the designator for "alkane" (no double or triple CC bonds).

C1	methane	C11	undecane	C30	triacontane
C2	ethane	C12	dodecane	C40	tetracontane
C3	propane	C13	tridecane	C50	tentacontane
C4	butane	C14	tetradecane	C60	hexacontane
C5	pentane	C15	pentadecane	C70	heptacontane
C6	hexane	C16	hexadecane	C80	octacontane
C7	heptane	C17	heptadecane	C90	nonacontane
C8	octane	C18	octadecane	C100	hectane
C9	nonane	C19	nonadecane		
C10	decane	C20	eicosane		

So, our first example of a straight chain compound (C_6H_{14}, $CH_3(CH_2)_4CH_3$) has six carbons in its longest chain, hence the name "hexane". What about the ring compounds? Well, our C_6 ring compound has 6 carbons, so it is a hexane. But it is cyclic, so it gets the prefix of "cyclo", to give cyclohexane. What are the names of the 2 compounds below?



A

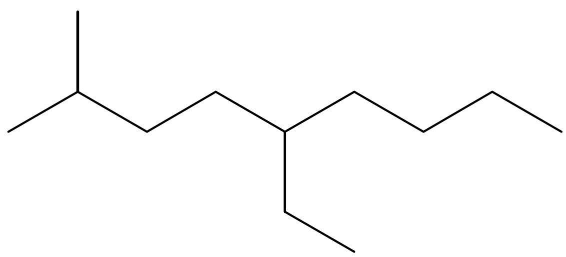


B

If you said octane and cyclobutane, you would be correct.

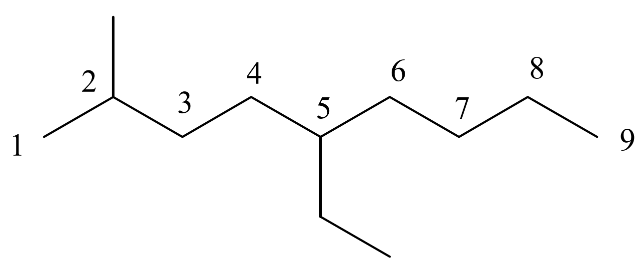
"So what's up with the numbers in some of the names?", you ask…To which I reply, "they tell you where the functional groups (substituents) are located." Okaaayyyy.

Consider the following hydrocarbon molecule…



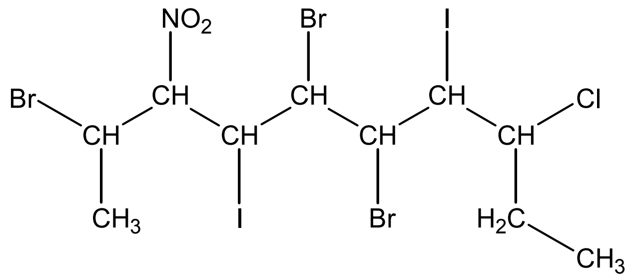
How do we name it? Very systematically.

1) Identify the longest continuous carbon chain, count how many carbons are in it, and that will be the root name…9 carbons = nonane.
2) Where does the first branch (substituent) occur? Start numbering the chain from that end



3) Name the appendage groups…methyl and ethyl
4) Put the appendage groups in alphabetical order…ethyl, methyl (di's and tri's don't count)
5) What is attached where? A methyl group on C-2 and an ethyl group on C-5…gives 5-ethyl and 2-methyl. (number and letters are separated by a hyphen, numbers are separated by commas)
6) Put it all together…5-ethyl-2-methylnonane.

Another example…



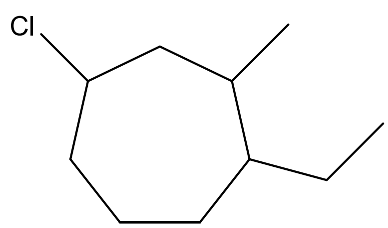
Follow the rules…2,5-dibromo-8-chloro-4,7-diiodo-3-nitrodecane

Iso, Sec and Tert. The above, iso, sec and tert, are three of the most misunderstood prefixes used in naming organic compounds. It is difficult to explain them without significant wanderings into isomerism. So, we will wait until we talk more about isomers until we deal with them.

Rings. As we saw, rings are named by attaching "cyclo" as a prefix…therefore pentane becomes cyclopentane …hexane becomes cyclohexane…etc. However, what about rings that have things (= functional groups, substituents) on them? Follow the rules…

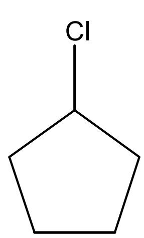
1) Identify the number of carbons in the RING…
2) Number the ring so that there is the lowest possible numbering system.
3) Alphabetize the substituents…
4) Put it together…

An example…



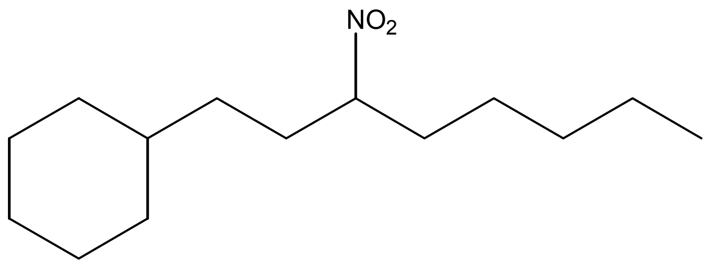
= 1-chloro-4-ethyl-3-methylcycloheptane

*a note: mono-substituted rings don't need numbers. For example…



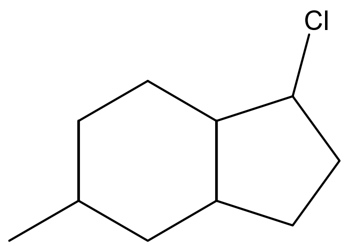
chlorocyclopropane
not
1-chlorocyclopropane

How about this?

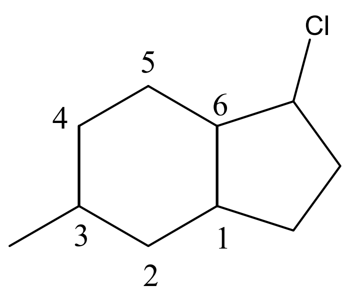


If the longest chain is bigger that the ring, then the chain is used as the base name. Therefore, this is 1-cyclohexyl-3-nitrooctane…not 3-nitrooctylcyclohexane.

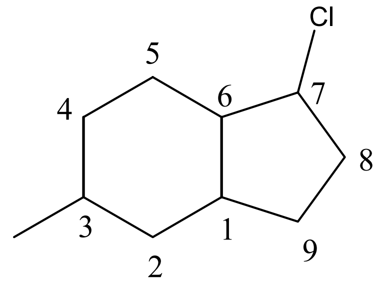
How about multiple ring systems? What do we call this one in IUPAC?



Starting at one bridgehead (place where two rings meet)…number to the other via the longest route (observing all other naming rules…)



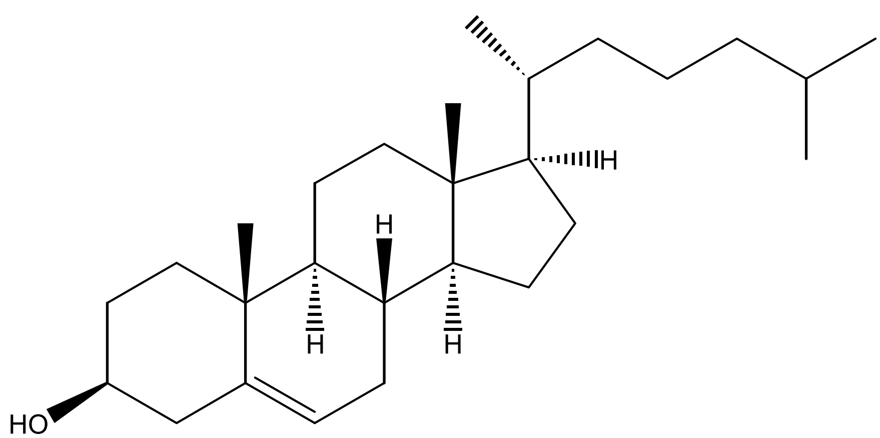
Continue to the original bridgehead via the next longest route…
Ad nauseum until all bridges are accounted for.



There are 4 carbons in the longest bridge [4]
…3 carbons in the next longest [3]

therefore: 7-chloro-3-methyl[4.3]bicyclononane

There is much more to learn about the nuances of naming organic compounds by the IUPAC conventions and even worse, by common names. The truth is, we as chemists are a lazy bunch. We use a combination of IUPAC and common names all the time. Can you imagine trying to write an IUPAC name for this beast, let alone use it in casual conversation?



…good thing we call it cholesterol.

We will add to our basic set of rules with more vocabulary and grammar as we encounter different classes of molecules (like for aromatic compounds), but this is more than sufficient to get us speaking in "organic chemistry".