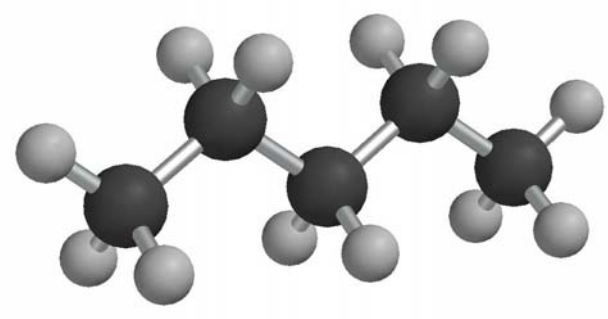
CHAPTER 2
ALKANES

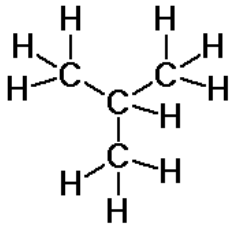
2.1 Introduction

Alkanes are organic compounds containing carbon and hydrogen with single bonds only. We will include compounds which contain a C bonded to a halogen also (C1, F, Br, I); these compounds are frequently referred to as halogenated alkanes. Recall that the geometry around C-H single bonds is tetrahedral and that the bond angle is 109.5^0, as shown for pentane below. Also remember that we can have free rotation around C-C single bonds.



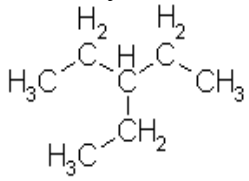
2.2 Naming of Alkanes

Frequently we will be looking at large, complicated organic molecules and we will want to refer to a small portion of that molecule by name without referring to the whole molecule. To take a simple example, let's look at the branched isomer of butane:



We can regard this molecule as being a chain propane molecule with a CH_3 group being substituted on the middle carbon atom and providing a branch point. Note that this CH_3 group is almost but not quite a methane molecule. There is one less H atom so that the CH_3 group can be bonded by its fourth bond to the propane chain. We call this CH_3 group a **methyl** group.

Similarly in the molecule:



We have a $-CH_2CH_3$ group being branching off of the middle C atom of a pentane molecule. Again the $-CH_2CH_3$ group is almost an ethane molecule except that one hydrogen has been removed so that the bond can be used to attach the group to the main chain. The $-CH_2CH_3$ group is called an **ethyl group.**

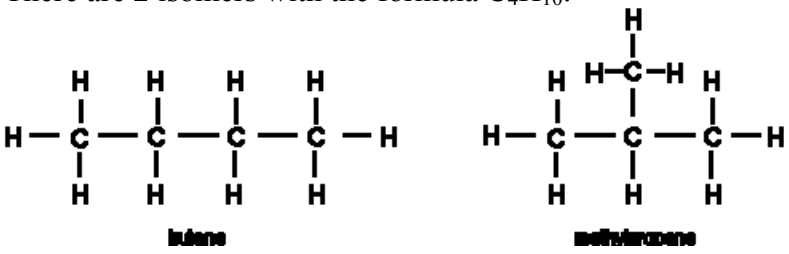
These are names for alkyl groups for any given number of carbons, but we will be concerned only with the names for chains ranging from 1-10 carbon atoms.

Number of C Atoms	Name
1	methyl
2	ethyl
3	propyl
4	butyl
5	pentyl
6	hexyl
7	heptyl
8	octyl
9	nonyl
10	decyl

The first four names (which are by far the most common) can be remembered by the mnemonic device:

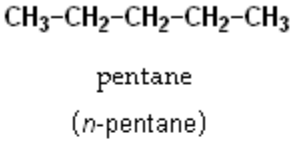
Methyl, ethyl
Propyl, butyl
After that,
It's all futile!

There are 2 isomers with the formula C_4H_{10}:



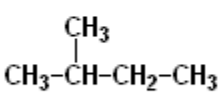
The unbranched chain isomer is called butane as indicated by the rules given above. The branched chain isomer was originally called isobutane, because it was an isomer of butane.

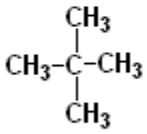
For the formula C_5H_{12} there are 3 isomers as shown below. The first molecule is the unbranched chain pentane; the second molecule has a methyl(-CH_3) branch off of a 4-C chain, and the third has 2 methyl(CH_3) groups coming off the middle C atom of the 3 carbon chain:



pentane

(*n*-pentane)





methylbutane (isopentane)

dimethylpropane (neopentane)

The first molecule is called pentane as before; the second isomer was called isopentane, and the third isomer was called neopentane because it was a new isomer (neo-is the Latin for new).

If we look at the table below however, we see that naming these isomers by simply putting prefixes in front of the name of the straight chain isomer will not be a very easy task for organic molecules containing a large number of C atoms. We will simply run out of names.

Chemical Formula	Number of Isomers
C_6H_{14}	5
C_7H_{16}	9
$C_{10}H_{22}$	75
$C_{15}H_{32}$	4347
$C_{40}H_{82}$	62,500,000,000,000

Clearly a more systematic way of naming molecule is necessary and organic chemists have developed such a system, called IUPAC nomenclature (International Union of Pure and Applied Chemistry). We will present the rules necessary to name alkanes in this unit, and will present additional rules for naming other functional groups in subsequent units. Although systematic names are used by professional chemists, it should be noted that most drug and food molecules are referred to by common non-systematic names. These names must simply be memorized.

Rules of Systematic Nomenclature

1. Name the longest (straight) unbranched carbon chain in the structure.

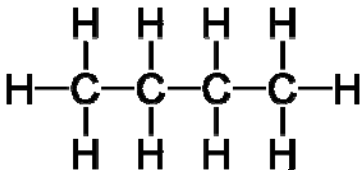
2. Preceding the name of the longest chain, write down in alphabetical order the names of each of the alkyl groups which are attached to the main chain.

3. If there are several groups of the same kind, list the group only once, using appropriate prefix: di- for 2, tri- for 3, tetra- for 4, penta- for 5, hexa- for 6, hepta- for 7, octa- for 8 to indicate how many of the groups there are.

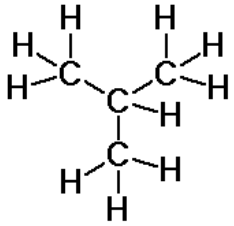
4. Assign a number, as a prefix, to each of the alkyl groups in the name to indicate the position of the group on the main chain. Start numbering from whichever end of the main chain results in the lowest sum of numbers.

.**Examples: Draw and name**

2 isomers of butane (C_4H_{10})

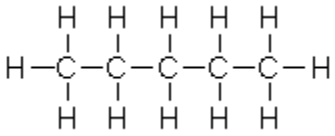


butane (as before)

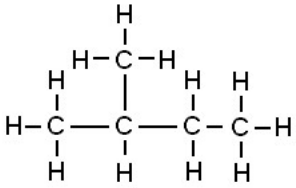


2-methylpropane

3 isomers with the formula (C_5H_{12})

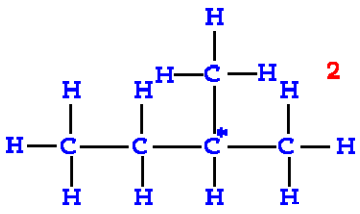


pentane (as before)

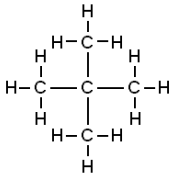


2-methylbutane
longest chain is 4 C's, so name compound as a derivative of butane with a methyl group hanging on 2nd C from the end

We might draw



as still another isomer and name it 3-methylbutane. Closer inspection shows that if we simply flip the molecule over from left to right we will have 2-methylbutane, which is the preferred name, since it has a smaller number.



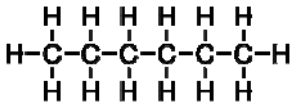
2,2-dimethylpropane

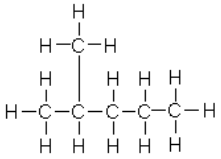
longest "straight" chain is 3C's so

name it propane; two methyl groups hanging off second C so we have 2,2-dimethylpropane

Note that IUPAC rules require that the number 2 be repeated to make it absolutely clearly that both methyl groups are on #2 C of the unbranched chain.

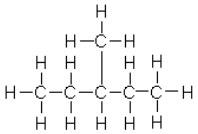
Draw 4 isomers with formula C_6H_{14}

Solution: 1)  hexane

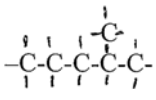


2) 2-methyl pentane. (We want to start numbering from left to right to keep the numbering as small as possible.

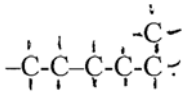
If we move the branch down one C on the main chain we have:



The name of this molecule is 3-methyl pentane and it does not matter from which end of the molecule we start the numbering.

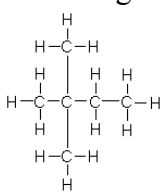
If we move the methyl group down another C on the main chain we have 

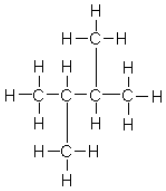
You might initially think this is a new isomer, 4-methylpentane, but closer inspection should make you realize this molecule is the same as 2-methylpentane, just flipped from left to right.

If we move the methyl branch 1 C further down the chain we have  .

Careful inspection of this conformation should reveal that it is NOT a branched isomer at all. It is just a different conformation of an unbranched 6 C hexane chain. It may be easier to visualize this if you take a pencil (or pen) and start from left to right. You can cover all 6 C atoms in one continuous stroke of the pencil.

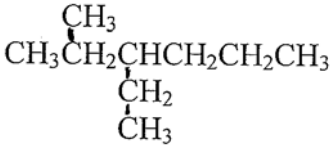
4) There are however two more isomers of C_6H_{14} which have two methyl groups branching off a 4 C unbranched chain.





2,2 dimethylbutane 2,3 dimethylbutane

Additional naming practice:



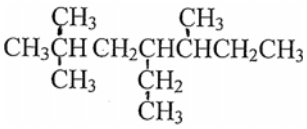
a)

The longest straight chain is 6 C's so name it hexane; add the branching chains in alphabetical order: ethyl and methyl. We still need to indicate where the ethyl and methyl groups are hooked on and that's where the numbers come in. Numbering from left to right we obtain:

3-ethyl-2-methylhexane Sum of numbers is 5

Numbering from right to left: 4-ethyl-5-methylhexane. The sum of the numbers is 9, so numbering from left to right is preferred.

Draw the line-bond notation for the above molecule.



b)Name:

Longest straight chain, ignoring branches, is 7 carbons.

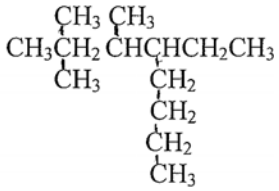
We have 3 methyl groups and one ethyl group branching off the main chain so our in front we have ethyl trimethyl

Now add the numbers, try starting from either end (then add the sum of the numbers).

Numbering from left to right we get 4-ethyl-2,2,5-trimethylheptane. Sum of #'s is 13

Numbering from the right to left we have 4-ethyl-3,6,6-trimethylheptane.Sum of #'s is 19
First answer is correct name because the sum of numbers is smaller.

c)Name



At first glance it might appear that the longest chain(reading straight across) has 6 C, but look again and notice there is a 4 C branch on C #4 (from the left). This "branch" is longer than the 2 C chain continuing horizontally. Since free rotation allows putting the chain in whichever direction we wish, the longest unbranched chain contains 8 C atoms

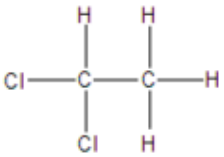
Numbering from left to right we have:
4-ethyl-2,2,3-trimethyloctane. Sum of numbers is 11
Number from right to left we have
5-ethyl-6,7,7 trimethyloctane. Sum of numbers is 25
First name is the correct one.

Naming alkanes with halogens

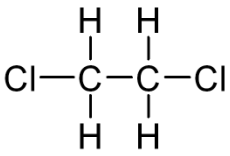
In naming a molecule which contain halogens (F,Cl,Br, and I) we treat the halogen just like an alkyl group and indicate its presence with the following names:

fluoro	for	F
chloro	for	C1
bromo	for	Br
iodo	for	I

Older common names for simple halogenated compounds often use the ionic form of the halogen name i.e. fluoride, chloride, bromide, and iodide even though no ionic bond is present.
CH_3Cl is named chloromethane. The older name is methyl chloride.
CH_3Br is named bromomethane. The older name is methyl bromide
.
Let's look at some examples:
a)Two molecules with which we introduced the concept of structural isomers:



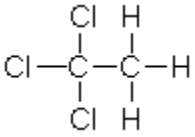
1,1-dichloroethane



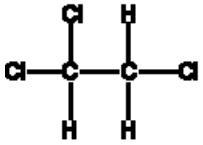
1,2-dichloroethane

The longest carbon chain in both cases is ethane and in both cases there are two chlorine atoms so name them both dichloroethane. However in the first case both C1 atoms are on the same C atom so call it 1,1-dichloroethane. In the second molecule the C1 atoms are on different carbon atoms so we indicate that as 1,2-dichloroethane.

b)Two isomers with the formula $C_2H_3C1_3$

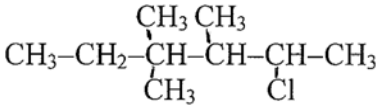


1,1,1-trichloroethane
(not 2,2,2-trichloroethane
and not 1-trichloroethane)



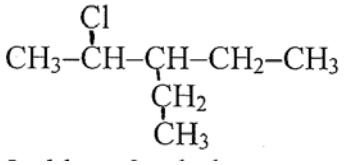
1,1,2-trichloroethane
(not 1,2,2-trichloroethane)

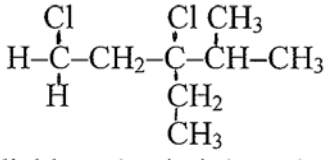
c) A molecule with both alkyl and halogen groups



Numbering from left to right: 5-chloro-3,3,4 trimethylhexane Sum of numbers is 15
Numbering from right to left: 2-chloro-3,4,4-trimethylhexane Sum of number is 13.
Numbering from right to left gives the correct name.

d)

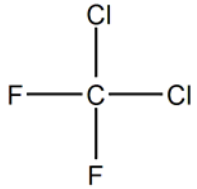




2-chloro-3-ethylpentane 1,3-dichloro-3-ethyl-4-methylpentane
What would the numbering be if we numbered from right to left?

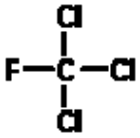
Examples with practical uses:

Freons



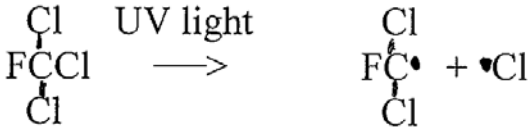
Dichlorodifluoromethane
(Freon12)

chlorotrifluoromethane
(Freon13)

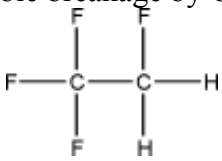


trichlorofluoromethane
(Freon 11)

Freon 12 and other Freons have been used as the gases in refrigerators and air conditioners, but when they escape to the upper atmosphere, UV radiation can break the C-Cl bond and produce Cl free radicals (molecules with unpaired electrons) which can then destroy ozone in the upper atmosphere.

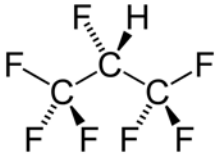


Chlorofluorocarbons(CFC's) were phased out in developed countries for spray cans in 1978, for refrigerators and air conditioners in 1995, and for medical inhalers (**metered dose inhalers** or MDI's for inhaled drugs such as **albuterol**) as of 2008. They have been replaced with hydrofluoroalkanes (HFAs) 134a and 227 which are *less* damaging to the ozone layer. (The hydrofluoroalkanes are less damaging to the ozone layer because the C-F bond is not as susceptible breakage by UV radiation as the C-Cl bond.)

HFA 134a has the structure 

and the systematic name 1,1,1,2-tetrafluoroethane

HFA 227 has the wedge and dash structure

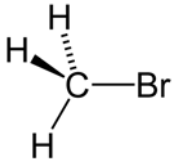


and the systematic name 1,1,1,2,3,3,3-heptafluoropropane.

Notice that both of these molecules contain only F halogen atoms and no Cl atoms. The C-F bond is much more resistant to UV light than the C-Cl bond. The substitution of HFAs for CFCs is more complicated than you might think and has required extensive research in the last two decades. The HFAs are more expensive to produce and large scale testing of efficacy and toxicity of the newly reformulated inhalers was required by the FDA. The cost of metered dose inhalers (MDIs) using HFAs are substantially more expensive than the old inhalers using CFCs.

Two albuterol inhalers reformulated with HFAs.

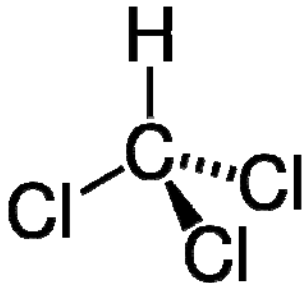
Bromomethane (Methyl bromide)



IUPAC: bromomethane
Common: methylbromide

Bromomethane (methyl bromide) has been used as a specialized soil fumigant, especially for growing strawberries. It is extremely toxic and great care must be taken in applying it. Methyl bromide is also a very potent ozone destroyer and there have been calls for taking it off the market for many years.

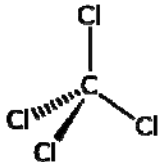
Trichloromethane(chloroform)



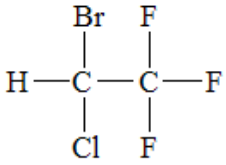
Trichloromethane (chloroform) was one of the earliest general anesthetics (a molecule which induces sleep as well as analgesia). It was administered by breathing the vapors of liquid chloroform and was first used during childbirth in 1847. It competed strongly with ether for the next 60 years as the general surgical anesthetic of choice. It has a sweet smell and is much less flammable and less irritating than ether, but the risk of putting the patient to sleep permanently is higher than for ether. Lethal overdose with chloroform was all too frequent and it could cause cardiac arrhythmias. Accumulated data published in 1934 showed that deaths from chloroform anesthesia were over four times as frequent as those with ether anesthesia (about 1 in 3000 for chloroform vs 1 in 14,000 for ether anesthesia). It is no longer use as an anesthetic.

It continued to be used in some cough suppressants and toothpastes and other cosmetics until such use was banned in 1976 based on data from rats that it could cause birth defects and liver cancer. Current exposure in the US is very small, primarily from chlorinated water reacting with organic compounds in the water to form trace amounts of chloroform in drinking water.

Tetrachloromethane(carbon tetrachloride)



Tetrachloromethane(carbon tetrachloride**) w**as commonly used as a drycleaning solvent in the first half of the twentieth century to remove grease and dirty from clothes.. It was also used in the synthesis of the Freon gases for refrigerators and air conditioners. Exposure to CCl_4 was associated with neurological, liver, and kidney damage and it was replaced as a dry cleaning solvent. Like the Freon molecules, CCl_4 can cause ozone depletion and its use has dropped dramatically.

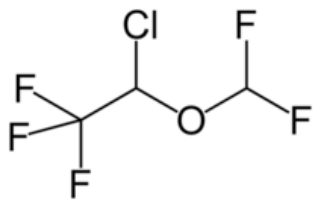


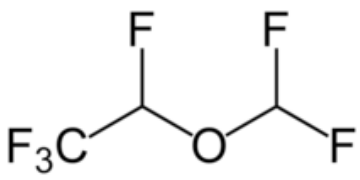
IUPAC: 2-bromo-2-chloro 1,1,1-trifluoroethane
Common: halothane

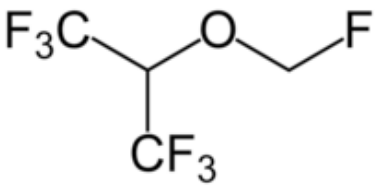
This molecule has the common name of **halothane**(suggest why!). It came on the market n 1956 and replaced ether as the anesthetic of choice because it was less irritating to the airway and it was not flammable. It did however have some adverse effects including cardiac depression (slowing of the heart rate) and rare (1 in 35,000) cases of hepatitis. It gradually lost "market share" to safer anesthetics.

Current inhalation anesthetics:

The current most commonly used inhalation anesthetics are halogenated ethers shown below which eliminate the flammability problem of ether and are generally less irritating to the airway than ether.





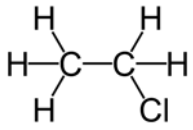


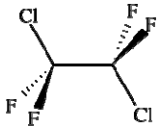
Isoflurane **Desflurane** **Sevoflurane**

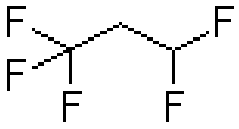
The mechanism of action of general anesthetics is poorly understood, is very complex, and probably involves many different factors. They appear to inhibit movement of the action potential along neurons as well as activating or inactivating a wide variety of neuronal receptors.

Topical anesthetics that work by chilling the skin surface

Name the following three molecules:

a) 

b) 

c) 

1 chloroethane
ethyl chloride

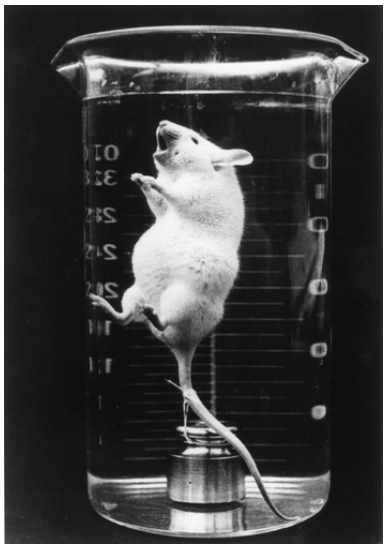
1,2-dichloro-1,1,2,2-tetrafluoroethane

1,1,1,3,3-pentafluoropropane

a)The first molecule has the common name ethyl chloride and has been used as a mild topical anesthetic while doing minor surgeries (e.g. removing a deep splinter). It has a low boiling point (12 ^{o}C) and boils off the skin (at 37^{o}C), lowering the skin temperature in the process and decreasing pain sensation. It is occasionally used as a recreational inhalant. Its use is decreasing..
b)The second molecule, 1,2-dichloro-1,1,2,2-tetrafluroethane, is marketed under the trade name, Frigiderm, works by a similar mechanism. It has a boiling point of 4^{o}C.

c) The third molecule, 1,1,1,3,3-pentafluoropropane, is marketed under the name Gebauer's Spray and Stretch. It is marketed for reducing pain of sprains. (Boiling point = 14^{o}C)

Perfluoroalkanes (completely fluorinated C chains) are liquids which dissolve large amounts of oxygen while remaining biologically inert. Such fluids were the basis for the oxygenated liquid in the movie The Abyss. Perfluoroalkanes have been investigated for filling the lungs of premature infants with respiratory distress syndrome. Clinical trials of one such liquid (Liquivent) were disappointing and it was not approved for market. Perfluorochemicals are also accumulating in the environment due to their invertness, albeit in small concentrations. They can accumulate in the fat of animals (including humans). Although their short-term toxicity appears to be low, long term data is minimal and there is increasing concern about the long term biological effects of perfluorochemicals accumulating in the body.



Perfluorochemicals have also been investigated for their use as artificial blood which could be used instead of real blood for blood transfusions. Perfluorochemicals would have the advantage of not having to match blood types and would not require testing for viral contamination with HIV and hepatitis which are necessary for blood transfusions. More recent research has been done on an emulsion of perfluorochemical, water, and lecithin) with the trade name Oxygent ^{TM}. There is definitely a demand for a blood substitute, but that product has not yet been widely marketed.

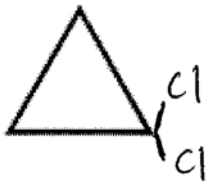
2.3 Cyclic Alkanes

We can bring an C chain around to its starting point and form a cyclic ring. We can form rings of different sizes. Let's look at each in detail.

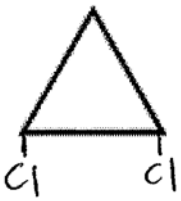
Cyclopropane 

We mentioned the fact that in regular alkanes the bond angle for single C bonds is 109.5^{o}. What is the bond angle in a 3-membered cyclic ring? 60^{o}. That's 49.5^{o} different from the bond angle that C prefers and as you will note I have used springs to make my model; if we tried putting wooden pegs in, we'd bust them because the holes were set for 109.5^{o}. As a result cyclopropane decomposes very easily and is very unstable; in fact, it's not only unstable, it's explosive; and yet at one time it was used as a general inhalation anesthetic; can you imagine what would have happened to your patient if that cyclopropane had exploded? You know that old story about how all the king's soldiers and all the king's men couldn't put Humpty Dumpty together again.

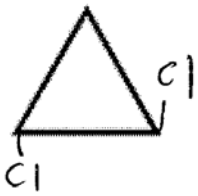
In the previous we talked about cyclopropane we mentioned the fact that geometric isomers (cis- trans isomers) can occur in cyclopropane ring even though there is no double bond. This turns out to be true for rings in general. To review it lets draw all the isomers that have 2 C1 atoms substituted on a cyclopropane ring and we'll name them.



1,1-dichlorocyclopropane



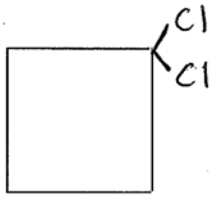
cis-1,2-dichlorocyclopropane



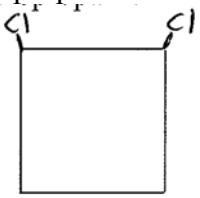
trans-1,2-dichlorocyclopropane

Note that the last two isomers have identical names except for the cis and trans out front.

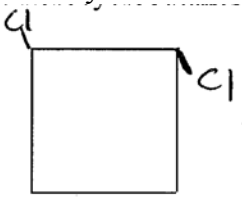
Cyclobutane-4-membered cyclic ring. It is to be expected that the bond angle would be 90^o while it would prefer to be 109.5^o. (The actual structure is a bit kinked and not exactly square, but we won't worry about this.) Cyclobutane is unstable and explosive although not quite as bad as cyclopropane. We can have geometric isomers in cyclobutane rings analogous to the isomers we had with cyclopropane; in fact we can have even more than we did for cyclopropane. Let's look at all the dichlorocyclobutanes:



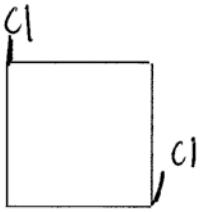
1,1 dichlorocyclobutane



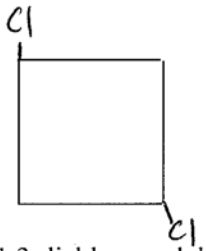
cis-1,2-dichlorocyclobutane



trans-1,2-dichlorocyclobutane



cis-1,3-dichlorocyclobutane

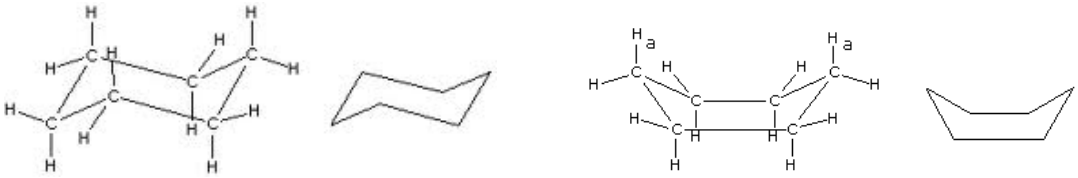


trans-1,3-dichlorocyclobutane

Cyclopentane is a 5-membered cyclic ring; bond angle is 108^o which is only 1^o off from what a normal C-C-C bond angle wants to be; cyclopentane is stable molecule, unlike cyclopropane and cyclobutane. The C atoms are essentially in one plane (one C atom is just a bit out of plane to improve the bond angle). Geometric isomers are possible with cyclopentane. Try drawing all the isomers of dimethyl cyclopentane. named below.

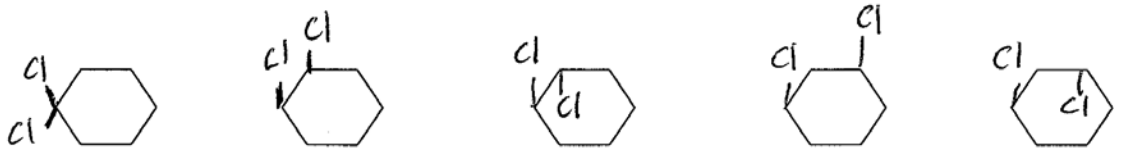
1,1 dimethyl cyclopentane | cis 1,2 dimethyl cyclopentane | trans 1,2 dimethyl cyclopentane | cis 1,3 dimethyl cyclopentane | trans 1,3 dimethyl cyclopentane

Cyclohexane is a 6-membered ring. In the previous ring structures I've drawn the molecules as being flat; that is, all the C atoms are in one plane of the paper. If this were true for cyclohexane, it would be in an hexagonal conformation with bond angles of 120^{o} which is considerably larger than the 109.5^{o} bond angle which it would prefer. In fact the bond angles in cyclohexane are 109.5^{o}. The molecule achieves this bond angle by getting a little kinky. Some organic chemist with an overwrought imagination called the two forms **chair conformation** and **boat conformation.**

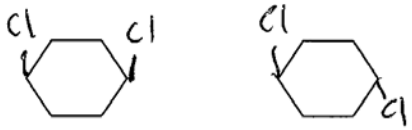


chair boat

Note that we can still have cis and trans isomers in cyclohexane ring, although its a little harder to see. For writing isomers we will go ahead and draw the cyclohexane molecule as a flat hexagon. Let's go through and draw all the isomers of dichlorocyclohexane.



1,1-dichloro-cyclohexane | cis 1,2 dichloro- | trans 1,2 dichloro- | cis 1,3 dichloro- | trans 1,3 dichloro-



cis 1,4 dichloro- | trans 1,4 dichloro-

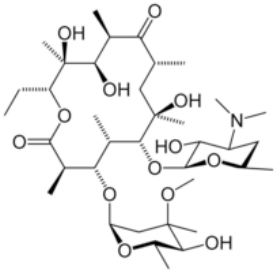
Note that even though even though the drawings may make most of Cl atoms look "outside" the ring and one of them "inside" the ring, this is just an artifact of the drawings.

Larger rings. As one increases the size of rings to 7 or more atoms in the ring, there is increased flexibility within the ring which allows the individual C atoms to achieve their desired bond angle (109.5 for single bonds) or something very close to it. For this reason

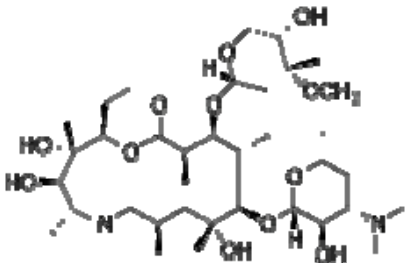
most rings with 7 or more atoms are usually stable, at least as far as bond angle stability is involved. Thus cycloheptane and larger rings are stable (but not flat!) molecules.

Cyclooctane

Some molecules with very large rings act as antimicrobial agents. The common antibiotic erythromycin has a 14-membered ring, as well as several 6-membered rings. The closely related antibiotic azithromycin has a 15-membered ring and two 6-membered rings (drawn flat in this diagram).

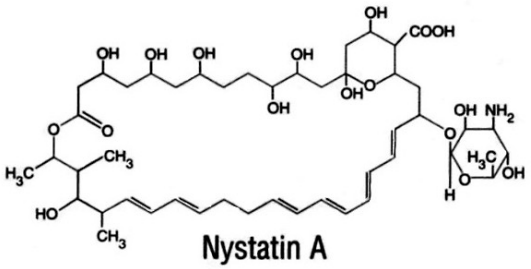


Erythromycin

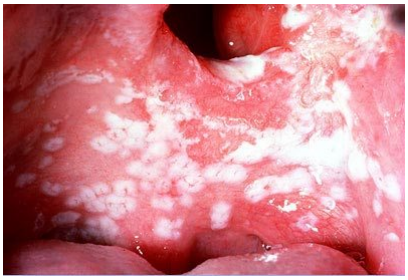


Azithromycin

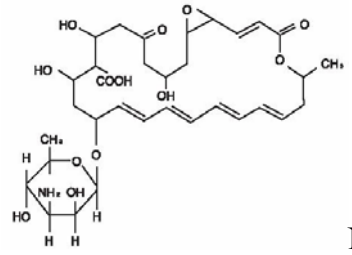
Some antifungal molecules dissolve into the fungal cell membranes. The large ring is thought to create a "hole" in the fungal membrane allowing the contents of the fungal cell leak out, thus eviscerating the microbe. Examples of drugs which act by this mechanism are Nystatin which is used to treat epidermal fungal infections such as **thrush.**



Nystatin A



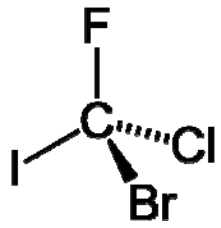
Another antifungal, natamycin, is used for treating fungal infections as well as a mold inhibitor, especially for dairy products. (Notice the presence of the epoxide ring, 6-membered ring, as well as the large ring in natamycin.) Based on your knowledge of the stability of cyclopropane, comment on the stability of the epoxide ring.



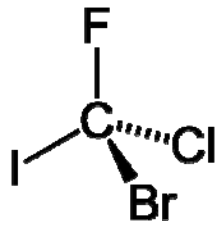
Natamycin

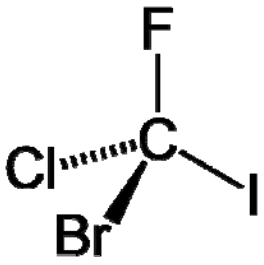
2.4 Enantiomeric Isomers

There is an additional type of isomer that can exist when we have an atom with 4 different groups attached to that atom in tetrahedral geometry. Consider a methane molecule with a fluorine, chlorine, bromine and an iodine atom bonded to it: bromochlorofluoroiodomethane. In wedge and dash notation we have.



If we take the mirror image of this molecule we will have the molecule on the right::





Original mirror image molecule

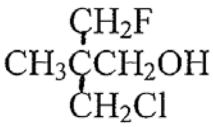
We might think that these are identical molecules, but if we make the real structures and try to align them we see that we can never line up all the atoms. If we rotate the mirror image molecule to line up the F-C-I atoms we find that the Br atom is now pointing back into the paper (i.e. it is the dashed form) and the Cl atom is pointing out of the plane of the paper towards us (i.e. it is now in the wedge form). No matter how we rotate the mirror image molecule it cannot be aligned with the original. The mirror image **is non-superimposable.**

This is somewhat analogous to taking the mirror image of a right hand glove. The mirror image of a right hand glove is a left hand glove, and although a left hand glove is clearly very similar to a right hand glove, it is not identical.

Non-superimposable mirror image molecules can occur whenever a molecule has one or more C atoms with 4 different groups bonded to it.

An atom (usually, but not always C) with 4 different **groups** bonded to it is called a **chiral center** or (in older terminology) an **asymmetric C atom**. *(The term chiral is pronounced kiral (rhymes with viral) and comes from chiros-Greek for hand, based on*

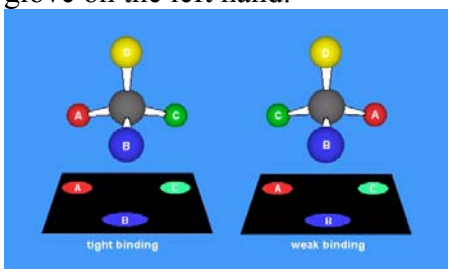
the right and left hand glove analogy. This root also shows up in the word "chiropractor")
[example]
We have to look at all 4 **groups** attached to a given C to decide whether it is a chiral center. Consider the molecule:



The center C has 4 C atoms attached to it, but it is still a chiral center because each of the C atoms it is bonded to is itself bonded to different atoms.

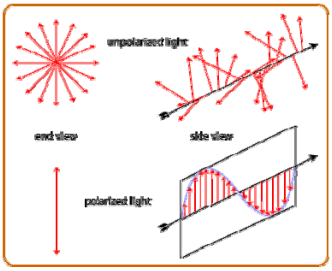
In general a molecule with a chiral center will have non-superimposable mirror image. These mirror image molecules are called **enantiomers** or in older notation **optical isomers.** More generally, molecules which differ only in the direction in which atoms are oriented in 3 dimensional space are called **stereoisomers**. Enantiomers and geometric isomers are two types of stereoisomers.

Enantiomers frequently have substantially different biological activity because they bind to receptors in the body that are also chiral. If one enantiomer molecule binds to complementary chiral binding site on an enzyme, the mirror image of the original molecule will not bind nearly as well, if at all. It would be like trying to put a right hand glove on the left hand.



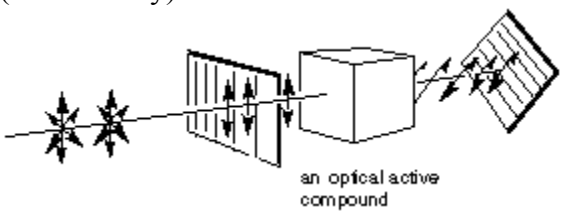
Enzyme Enzyme

Enantiomers also differ in the way they affect polarized light. Ordinary light has light vibrating uniformly in all different planes perpendicular to the direction it is moving. Polarized light is vibrating only in one plane.



Enantiomers differ in the way they affect polarized light that passes through them. When polarized light passes through a pure enantiomer, one enantiomer will rotate the plane of vibration (not the direction of the light!) to the right (+)(dextrorotatory), while the other

mirror image will rotate the polarized plane of vibration an equal amount to the left (-) (levorotatory).



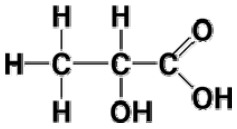
http://www.youtube.com/watch?v=QgA6L2n476Y

Two common notations besides + and - are used to distinguish between the two forms of optical isomers. In an older (but very common) notation D (for dextro) and L (for levo) are used to designate the two enantiomeric forms. In the other system the prefixes R(for rectus) and S (for sinister)are used to designate the two enantiomeric forms. The explanation of both notations is somewhat complex and will be omitted, but you should know that if you see the symbols +/-, D/L, dextro/levo or R/S in front of a chemical name, it means you working with one of 2 enantiomers. You do NOT have to figure out which structure is which in the R/S, D/L prefix system.

Practice Identifying the chiral centers (asymmetric Cs)

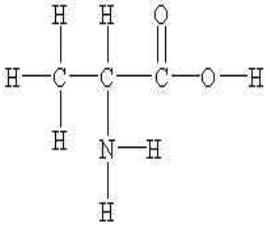
a)

Lactic Acid



We can check each of the three C atoms for chirality. Starting from left to right, the first C is clearly not chiral because it has three H atoms bonded to it. The second C atom *is* chiral because it has a methyl group, an OH group, a carboxylic acid group and a H bonded to it. Hence it is chiral. The last C is not chiral because it has only three groups bonded to it. Hence there is one chiral atom, the central C atom and there are + and -, or D and L (or R and S) forms for lactic acid. You do not have to decide which is which. The lactic acid that builds up in animal muscles is actually the pure L or + form. Bacterial cultures (such as that found in yogurt) produce primarily, but not exclusively the L isomer.

b)

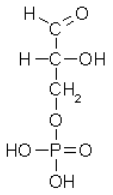


Alanine—a common amino acid

(Circle the amine and carboxylic acid groups.)

Likewise the first C (going from left to right) cannot be chiral because it has 3 H atoms; the middle C atom IS chiral because it has 4 different groups (a CH_3, an NH_2, a H and a CO_2H). The third C is not chiral because it only has 3 groups around it). Alanine can exists in two enantiomeric forms, most commonly referred to as the D and L forms. In general, the L form of amino acids are the most common and are the ones exclusively used to make proteins. D enantiomeric amino acids are found occasionally, such as in the amino acids found in bacterial cell walls.

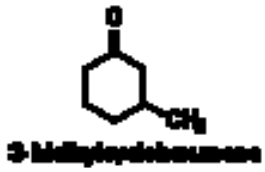
c)Glyceraldehyde-3-phosphate



Fischer
open-chain

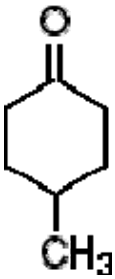
This molecule is present vertically rather than horizontally, but that should not cause too much problem. Hopefully you reach the conclusion that the middle C is the only chiral center. The D-enantiomer of this molecule is made when glucose is metabolized. *Label the aldehyde functional group.*

d)



This molecule gets a little trickier and it will probably be useful to draw the complete structure. You should reach the conclusion that the C of the carbonyl group cannot be chiral, nor can any of the other C atoms in the ring except the C bonded to the methyl group. That C is however bonded to 4 different groups: a methyl group and to the ring (twice, but from two different directions) and to a H atom (which is not explicitly shown in this shorthand notation). However the bonding clockwise around the ring is $CH_2CH_2CH_2C{=}O$ and in the other direction it is $-CH_2C{=}O$. Those bonds are different and hence 3-methylcyclohexanone exists as two enantiomers.

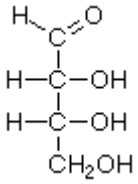
e) **4-methylcyclohexanone**



4-methylcyclohexanone

If you look at the structure of 4- methylcyclohexanone, you should see that the C bonded to the methyl group is symmetrically bonded within the 6-membered ring, so that it is NOT chiral.

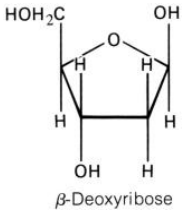
f)erythrose



Erythrose

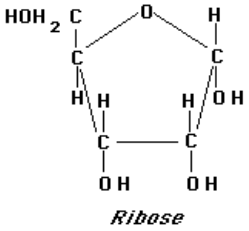
In the molecule erythrose, the aldehyde C cannot be chiral because it does not have four different groups. The next C has a H, OH, C=O, and $CHOHCH_2OH$ group bonded to it. The third C has a H, OH, CH_2OH, and CHOHC=O bonded two it. There are 4 different groups on both of the middle C atoms, so they are both chiral. The fourth C has two hydrogens bonded to it so it is not chiral. Multiple chiral atoms in a single molecule are in fact very common in biological molecules. They do make for a quite complex brew of **stereoisomers** that is beyond this text. Although we will identify chiral centers in molecules, we will not try to look at the complexities that result in molecules with multiple chiral centers.

Label chiral centers in the molecules below with a *.



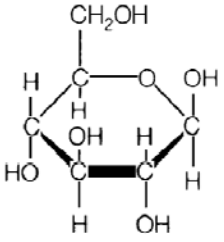
β-Deoxyribose

deoxyribose



Ribose

ribose



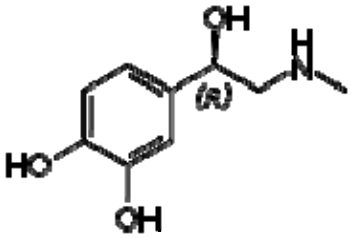
Glucose

Enzymes produce only 1 enantiomer of any possible pair, but synthetic organic chemists often produce a mixture of both enantiomers. A mixture of both enantiomers is called a **racemic mixture.** This is particularly important when drug molecules are synthesized. These drugs generally bind to **chiral receptors** and as a result one enantiomer usually binds the desired site better than the other, as we saw with DES in the previous chapter.

Pharmaceutical chemists have developed increasingly sophisticated drug syntheses that allow them to make pure enantiomers rather than racemic mixtures and newer drugs on the market are often pure enantiomers.

Some Medically important examples of enantiomers:

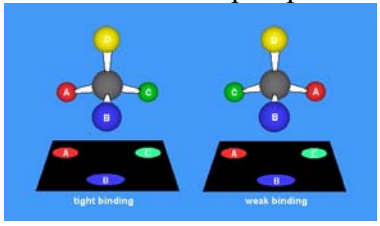
1)Epinephrine(adrenaline)



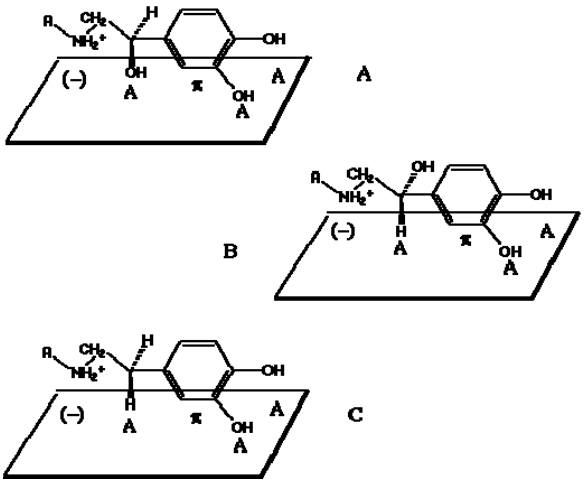
Epinephrine(adrenaline) How do the two differ in structure?

Epinephrine (adrenaline) acts as a neurotransmitter or hormone which binds to several different kinds of **adrenergic** receptors in the body and cause a large variety of physiological effects. The best known effect is the "fight or flight" phenomenon or "adrenaline rush" which increases heart rate and blood pressure. Epinephrine is used as a drug for the treatment of anaphylactic shock where it increases heart rate and blood pressure. It is commonly added to local anesthetic injections to promote vasoconstriction at the injection site, thereby reducing the amount of local anesthetic that gets into the blood stream.

Epinephrine contains a chiral center in its structure. Can you find it? The naturally occurring form in organisms is the (D) R (-) enantiomer. When epinephrine is used as a drug, the routine organic synthesis results in a **racemic mixture**. The (+) S enantiomer does not typically bind as well to adrenergic receptors nor produce as much activity but its presence in the racemic mixture doesn't appear to be a clinical problem either. Organic chemists are getting better at synthesizing pure enantiomers in mass quantities and commercial epinephrine is now typically the pure D enantiomer.

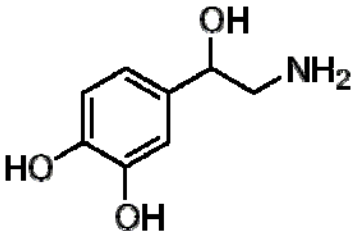


The diagram A below shows that the D enantiomer of epinephrine binds to 3 **A** sites aligned on the plane to attract the polar OH groups. In B, the L isomer only binds the two OH on the ring, and hence binding is not as good. In C, dopamine does not have any OH group at the first A site on the left and it also does not bind as well.



dopamine

2)Norepinephrine



Norepinephrine is another important neurotransmitter in the body.

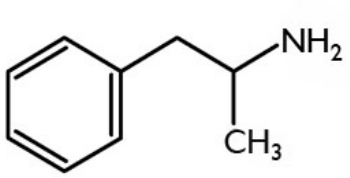
How do the structures of epinephrine and norepinephrine differ? How are they similar? Label any chiral centers in norepinephrine.

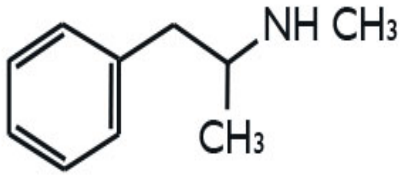
3) **Dopamine**

Dopamine is another neurotransmitter with a large variety of actions on different receptors in the brain. It is involved in regulating motor activity, motivation, and the pleasure response and overproduction of dopamine in the "pleasure center" of the brain can lead to addiction. High dopamine levels in the chemoreceptor trigger zone (CTZ) can

cause nausea and vomiting. It has a structure similar to epinephrine and norepinephrine. Does it have a chiral center? Why or why not?

4)Amphetamine (sold as trade name product Adderall) and methamphetamine, formerly used as an appetite suppressant and as a stimulant ("cognitive enhancer")by truck drivers, pilots, and students(!), is currently approved by the FDA for use in treating attention deficit and hyperactivity disorder (ADHD). Methamphetamine has an extra methyl group added to the amine group in amphetamine.





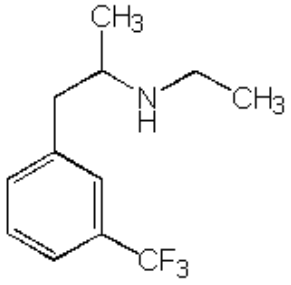
Amphetamine Methamphetamine

As originally marketed, amphetamine contained both D and L isomers, with only the D isomer having significant activity. Increasingly sophisticated organic chemistry techniques have produced the pure D enantiomer which is available in a sustained release form of amphetamine (Adderall).

Methamphetamine has become an "upper" of choice on the street drug circuit because of the huge "high" it causes. This should not be entirely surprising given its similarities to epinephrine. Meth also contains a chiral center.

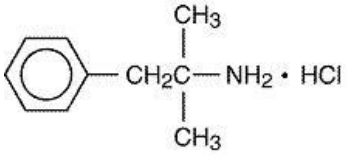
Plant an * by the chiral center of both molecules. Is the chiral center the same C as in epinephrine and norepinephrine?

5) Fenfluramine(Pondimin)



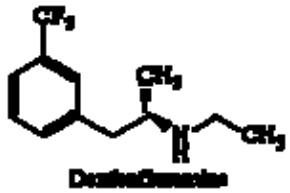
Fenfluramine was a drug that was a very popular appetite suppressant in the late 1980's and early 1990's. As originally marketed, it contained a racemic mixture of both D and L fenfluramine enantiomers. While D-fenfluramine (or dexfenfluramine) suppressed the appetite, its mirror image molecule caused drowsiness.

To counteract the drowsiness, the **racemic** fenfluramine was combined with a drug called **phentermine** a mild "upper", which has been used by itself as a weight loss drug. **Phentermine** stimulates the sympathetic nervous system (fight or flight) to counteract the drowiness caused by L-fenfluramine. The combination was marketed as **fen-phen** and was a huge product in the weight loss industry in the early 1990's. In 1997 reports of heart defects, some of them fatal, in fen-phen patients started being reported to the FDA and in September of 1997 fenfluramine was pulled off the market. Lawsuits started immediately and are still ongoing, with settlements in the billions of dollars.



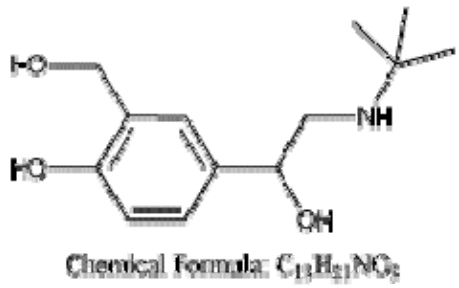
phentermine

As with the case of Adderall, synthetic organic chemists developed a chiral reaction pathway to make pure dexfenfluramine, which was marketed as Redux in 1996, just a year before the revelations about heart valve defects. Redux was associated with heart valve defects just as was the racemic mixture of fenfluramine and was also removed from the market place.

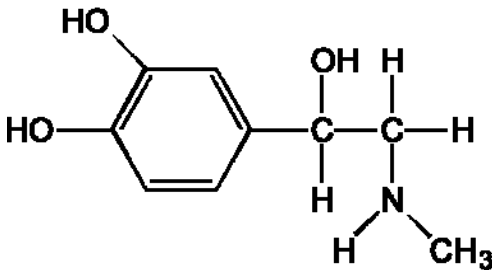


6) Albuterol

Albuterol is a very common asthma medication. Although there are differences, notice the similarities in the structure of albuterol and epinephrine. In fact albuterol acts to activate epinephrine receptors specifically in the lung to cause broncodilation.



Albuterol



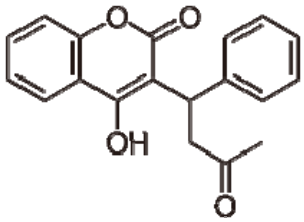
epinephrine

R albuterol (levo albuterol) is the enantiomer which causes bronchodilation desirable in asthmatics. S albuterol (dextro albuterol) appears to be relatively biologically inactive.

Label the chiral center in albuterol

The current albuterol on the market is a racemic mixture of + and - albuterol. Pure (-) L albuterol is available as levalbuterol (Xopenex) but has not been found to be better than the racemic mixture by most clinicians and its cost is about six times the racemic mixture.

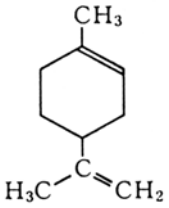
7) Warfarin(Coumadin) is a very common blood anticoagulant. (Warfarin is the generic name; Coumadin is the trade name of a specific manufacturer)



Commercial Coumadin is a racemic mixture of R and S(D and L) enantiomers. Although both enantiomers are anticoagulants, the S isomer is 3-5 times as active as the R isomer. Can you identify the chiral center?

8)Limonene

Limonene is one of the molecules responsible for producing the characteristic citrus smell of lemons and oranges. It is a byproduct from the orange juice and lemonade manufacturing and is used to provide the citrus smell in a wide variety of cleaning, degreasing, and cosmetic products.

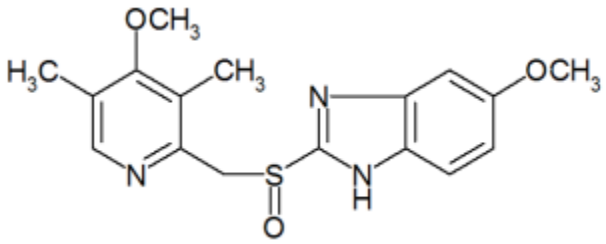


Limonene exists as two enantiomers. Can you find the chiral center?
R (+) limonene is the naturally occurring enantiomer in citrus oil. S (-) limonene has more of a pine resin smell.

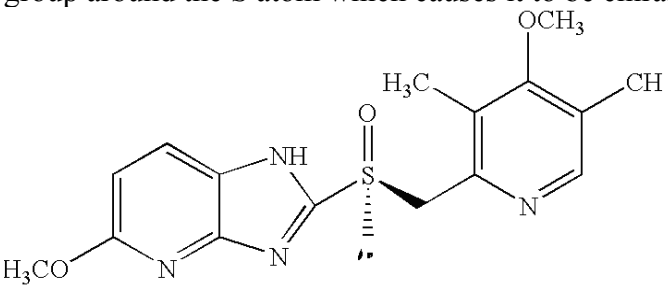
9)Omeprazole (Prilosec)

Omeprazole(Prilosec) is a **proton pump inhibitor(PPI)** that shuts down HCl secretion into the stomach and is used for the treatment of ulcers and *GERD(*gastroesophageal reflux disease, heart burn*).* It exists as a racemic mixture. The chiral center is different from the previous examples in that it is the S atom in the structure. This may seem strange because all of our previous examples of chiral centers were C atoms. C is by far

the most common **chiral center**, but there are other atoms that can show chirality and this is one example. The next apparent contradiction is that one needs to have 4 different groups on an atom for it to be chiral, and the S atom in omeprazole only has 3 groups bonded to it.



The contradiction is resolved if one looks closer at the actual Lewis dot bonding of the S atom and realizes that there is a non-bonding pair of electrons which is rarely if ever shown when its structure is drawn. This non-bonding pair of electrons constitutes a fourth group around the S atom which causes it to be chiral.



Omeprazole(Prilosec) is the racemic mixture of the two enantiomers. The clever organic chemists at AstraZeneca worked out a synthesis of the pure active S isomer and when the patent on Prilosec ran out, its manufacturer introduced esomeprazole (**Nexium)** which is the pure biologically active enantiomer of Prilosec and marketed it heavily. The es in omeprazole stands for the prefix S.

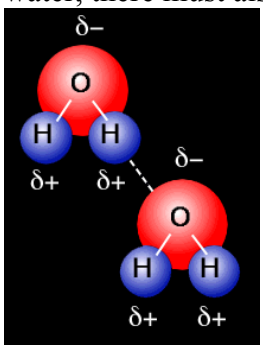
2.5 Solubility of Alkanes

We learned in the chapter on solutions that "like dissolves like": polar and ionic compounds are generally soluble in polar solvents like water, but not in non-polar (covalent) solvents like gasoline, oil, and (more biologically important) fat. Likewise predominantly non-polar (covalent) compounds are soluble in non-polar solvents, but not in polar solvents such as water.

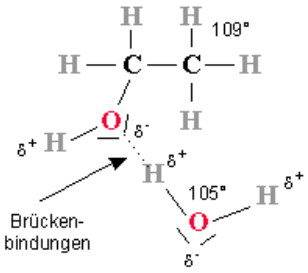
The solubility of various organic molecules such as drugs, vitamins and hormones is of great physiological importance and we will be looking in substantial detail about the solubility of various biologically important organic molecules.

Recall that there are attractions between water molecules based on the attraction between δ+ on the H atoms of one water molecule and δ- on the O of another water molecule.

These attractive forces are called **hydrogen bonds**. For a substance to be soluble in water, there must also be attractions between that solute molecule and water molecules.



When we dissolve a polar or ionic compound into water, the same sort of attraction can occur; e.g. when we dissolve ethanol (ethyl alcohol) in water. This attraction allows ethanol to dissolve freely in water.



A similar situation occurs with methanol dissolved in water. Draw the arrangement that shows attractions between a methanol molecule and water.

A similar situation occurs with ammonia(NH_3) dissolved in water. Draw the arrangement that shows attractions between an ammonia molecule and water.

If we look at the alkanes, there are no polar bonds in molecules containing only hydrogen and carbon and hence there is no attraction between alkane molecules and water molecules. Do you think any of the alkanes are going to be soluble in water?

However solubility is not a black and white thing. Look at what happens to solubility (at 20^{o}C) in the following series of molecules, each containing one polar OH group.

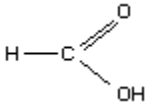
Alcohol solubility in water

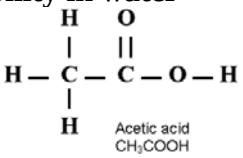
Solubility in H_2O:	CH_3OH	CH_3CH_2OH	$CH_3CH_2CH_2OH$
	complete(∞)	complete(∞)	complete(∞)

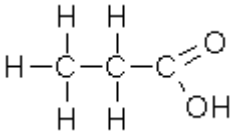
Solubility in H_2O:	$CH_3CH_2CH_2CH_2OH$	$CH_3(CH_2)_3CH_2OH$	$CH_3(CH_2)_4CH_2OH$
	12.5g/100ml	2.5 g/100ml	0.6 g/100 mL

(∞ is used as shorthand for completely soluble)

Carboxylic acid solubility in water







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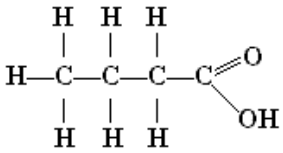
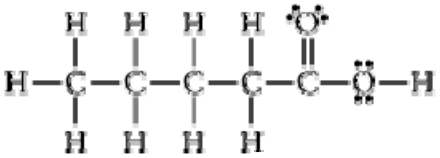
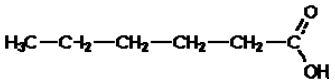






5.62 g/L 3.7 g/L 0 .4 g/L

Carboxylate ions and ammonium ions

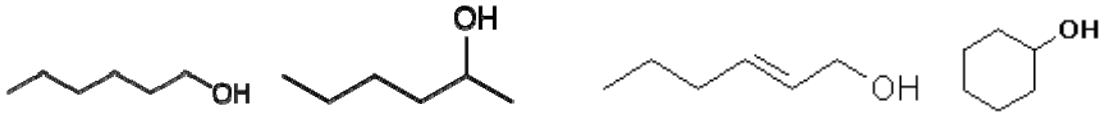
Carboxylate ions and ammonium ions tend to be completely soluble in water up to a length of approximately 16-18 C atoms. Evidently ionic groups are substantially more hydrophilic than polar O-H and N-H groups. Conversely **compounds with ionic groups are not at all soluble in very non-polar solvents such as hexane**, gasoline, and biological membranes.

The water solubility data of compounds above can be combined with data for some other polar functional groups as shown in the chart below

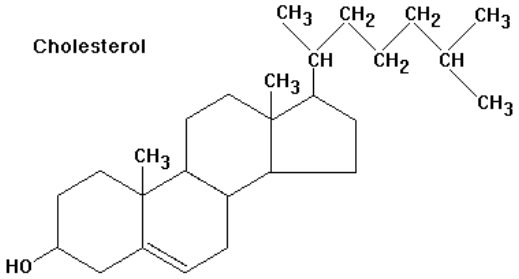
Number of C's	1	2	3	4	5	6
Functional group						
Alcohol	∞	∞	∞	12.5	2.6	0.6
Carboxylic acid	∞	∞	∞	5.62	3.7	0.4
Ketone	∞	∞	∞	35	4.7	1.4
Amine	∞	∞	∞	∞	∞	1.2
Amide	∞	∞	∞	16		
Carboxylate ion	∞	∞	∞	∞	∞	∞
Ammonium ion	∞	∞	∞	∞	∞	∞

∞ means completely soluble in water. Solubilities listed above are in g/L
(Data from CRC Handbook of Chemistry and Physics)

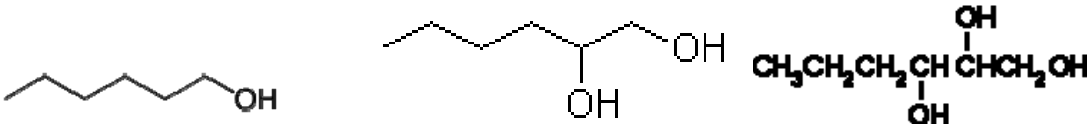
As a general rule of thumb we can observe that the polar groups listed in the chart can solubilize a non-polar chain up to a length of around four to five CH_2 units (including the C with the polar group).. The solubility is not affected significantly by the position of the polar group in the molecule or the presence of rings or C=C bonds.



All four of the above molecules have one polar OH group and a nonpolar chain 6 C atoms long and they all have low solubility in water, on the order of a gram/L. All of them are more soluble than cholesterol, with structure shown below. Cholesterol has one polar OH group and a non-polar C chain of 25 C atoms!

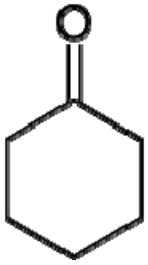


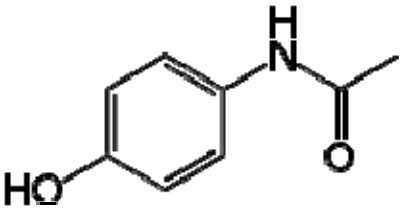
There are substantial variations in molecules with complex structures and real experimental data is always the final word, but we can make predictions on the solubility of a compound by counting the ratio of nonpolar CH_2's to polar functional groups. If the ratio is less than 4 it will probably be quite soluble in water (and the smaller the ratio, the more soluble it will be). Molecules with 5 or more CH_2 units per OH or other polar group will not be very water soluble, and the larger that ratio is, the less soluble it will be.



All of the above molecules have a 6 C chain but the first one has 1 OH group, the second molecule has 2 OH groups and the third one has 3 OH groups. Thus the nonpolar C/OH ratio in the first molecules is 6:1; the second molecule has a 6:2 or 3:1 C/OH ratio; the third molecule has 6:3 or 2:1 nonpolar/polar ratio. One can make the reasonable prediction that the first molecule will have low solubility in water, the second one will be quite soluble in water and the third one will be very soluble in water.

Predict the solubility of the following molecules in water:

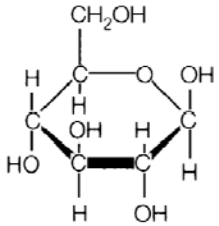




acetaminophen

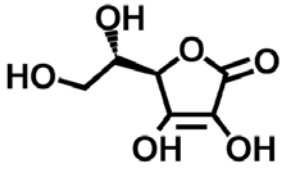
Answer: The first molecule has one polar ketone group on a 6-membered ring while the second molecule has 2 polar groups on the 6 membered ring. One will predict that the first molecule will have low solubility, similar to the previous cyclohexane with an OH group, while the second molecule will be quite soluble in water. Acetaminophen has 2 polar functional groups (OH and amide—treat the amide as one polar group). for 8 C atoms or a 8/2 = 4:1 ratio and would be predicted to be moderatelysoluble in water.

One can often predict the water solubility of complex biological and medically important molecules by looking at their structures and assessing the number of polar groups compared with the number of C's in nonpolar bonds. For example:



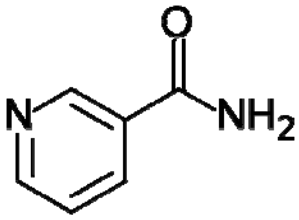
Glucose is the sugar found in blood and it is easy to see why it is very soluble in water. Every C has a polar OH group on it.

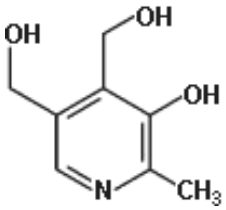
Water soluble vitamins



Ascorbic acid(Vitamin C)

Likewise ascorbic acid has a polar group on every C.

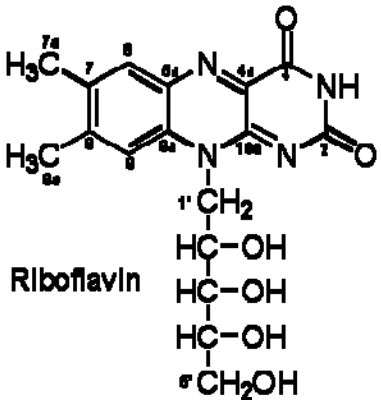


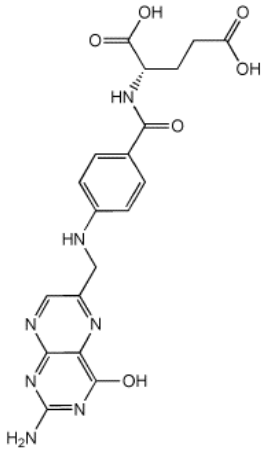


Nicotinamide(vitamin B3) pyridoxine(Vitamin B6)

Nicotinamide has a polar amide group and a polar N-C bond in the 6-membered ring and 6 C units in the ring, giving a 6:2 nonpolar to polar ration and a prediction that it will be soluble in water. Pyridoxine is even more polar with 3 polar OH groups, a polar C-N bond and 8 nonpolar C units.

Without trying to do a precise count of polar groups vs nonpolar units, you should be able to "eyeball" the structures of the molecules below and conclude that there are enough polar groups to makes these molecules quite water soluble.

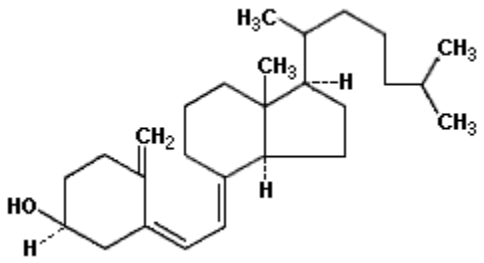




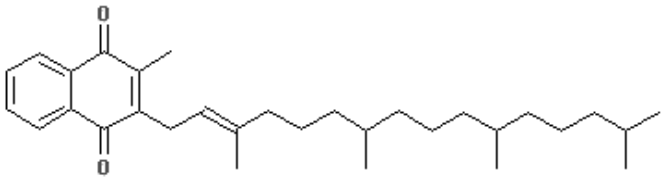
Riboflavin(B2) Folic acid

Ascorbic acid, nicotinamide, thiamine, riboflavin and folic acid are all classified as water soluble vitamins, with good reason.

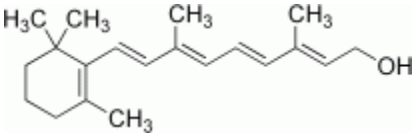
Fat soluble vitamins



Vitamin D_3



vitamin E



vitamin A (retinol)

Although the above three vitamins all have one or more polar groups, they have a much larger structure that is non-polar. Hence these molecules as a whole are not water soluble and are much more soluble in non-polar fat. They are in fact referred to as **fat soluble vitamins.**

2.6 Petroleum

Petroleum (crude oil) consists of a mixture of alkanes and alkenes (both unbranched, branched, and cyclic) of widely assorted lengths and boiling points. The boiling point of these molecules increases as the length of the chain increases as shown in chart below.

	Boiling point (^{o}C at 1 atmosphere pressure)
Methane	-182.77
Ethane	-88.6
Propane	-42
Butane	-0.5
Pentane	36
Hexane	68.7
Heptane	98.4
Octane	125.67
Nonane	150.82
Decane	174
Eicosane (20 C atoms)	343

(Source, CRC Handbook of Chemistry and Physics, 88th ed, 2007)

Even though the bonds in these alkanes are quite non-polar, there are very weak attractions (called **van der Waals attractions**) between molecules and as the molecules become larger and larger, these attractions between molecules become larger and result in increased boiling points.

These different molecules are partially purified by **fractional distillation** where lower boiling liquids are preferentially boiled off and separated from higher boiling substances. This process does not separate out pure compounds, but it does separate the crude oil into separate fractions with similar boiling points.

A brief summary of some of the fractions from a petroleum refinery is shown in the chart below

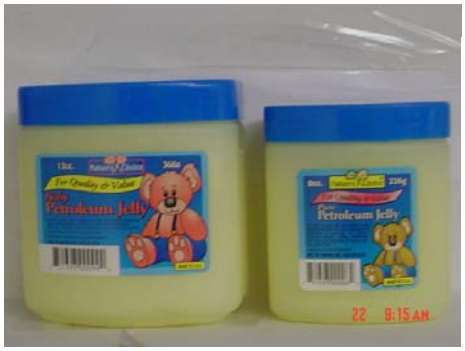
	C chain length	boiling point range
Gasoline	5-12	< 200 C
Kerosene	12-15	150-275
Diesel	10-19	200-350
Mineral oil	15-40	~300
Lubricating oil	20-40	>370
Asphalt	>40	very high

One of the most desirable properties of gasoline is that it does not actually ignite (burn) until a spark is applied. This property is measured by the octane number and the higher the octane number, the more resistant the gasoline is to premature ignition. Branched alkane chains and cyclic alkanes have higher octane values than unbranched chains. Given that gasoline is a major product from petroleum, a lot of reforming reactions are carried out in petroleum refineries to increase the % of branched and cyclic alkanes and hence to increase the octane value of gasoline fractions from the distillation.

Mineral oil consists of a mixture of alkanes from 15-~40C atoms that is commonly used (with the addition of fragrances) as baby oil. It is also used in some cold creams and ointments. It can replace the natural oils that may be removed from a baby's skin with routine cleaning and may reduce the irritation and rash from diapers by applying a non-polar barrier on the baby's skin which will not allow urine and feces direct contact with skin.

It is also occasionally used internally as a laxative to treat constipation. The non-polar mineral oil can coat the lining of the large intestine, inhibit water reabsorption in the intestine and thus increase the fluidity and volume of the bowel contents. There are other OTC treatments available and this use is not recommended by many doctors.
It can also be used to dissolve impacted ear wax.

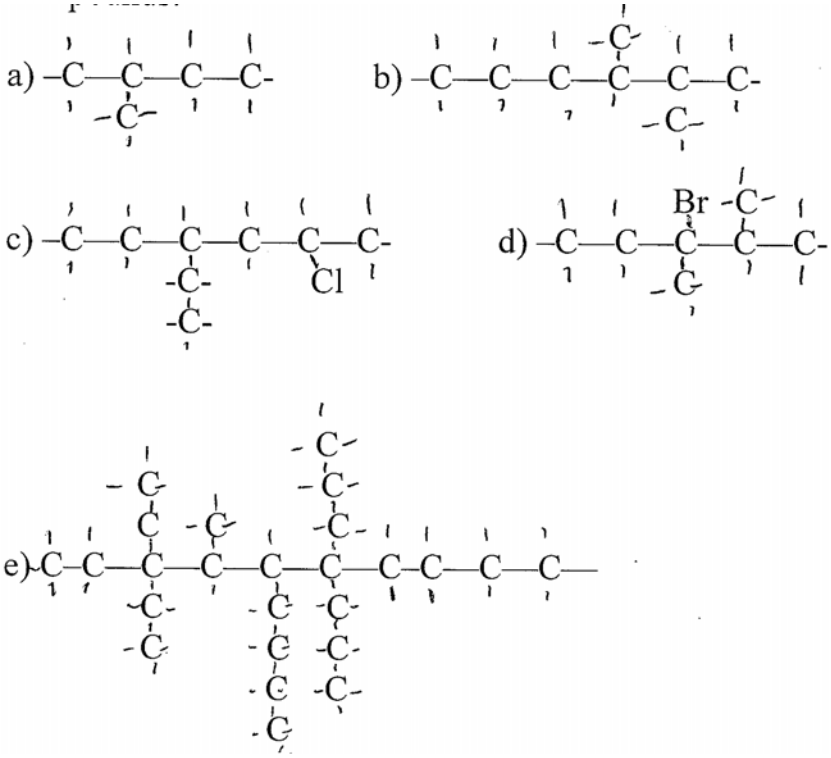
Petroleum jelly (petrolatum, Vaseline) is a semi-solid mixture of alkanes of slightly higher molecular weight than mineral oil (more than 25 C atoms) and is used in a similar fashion. It is also used as a component of some lip balms and moisturizers.



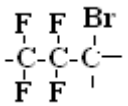
Some ultrasound gels

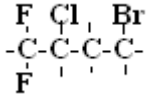
Alkane Study Guide

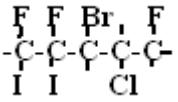
1. Give systematic names for each of the following chemical compounds:



f) 5 isomers with formula C_6H_{14} g) 4 isomers with formula $C_3H_6Cl_2$

h) 

i) 

j) 

2. Draw the structure for

   a) 2,3-diethyl-4-methylheptane
   b) 3,4,5-triethyl-5-propyldecane
   c) 2-methyl-3-ethyl-4-propyl-5-butyl decane
   d) 2,2-difluoroheptane
   e) 2,4-dibromo-1,3-difluorobutane
   f) 1,3-dichloro-2-iodopropane
   g) 1,1,2,2-tetrafluroethane
   h) 1,1,1,2,3,3 hexachloropentane
   i) 2,3,4-tribromo-5,5-dichloro-1-fluorooctane

3. Draw an example of a freon molecule. Where are freons used? Why are freons being phased out? How are the new replacements different from the older freons and why are they better? What abbreviation is used in referring to the older freons? Newer freons?

4. What were some of the primary problems with using chloroform as a general anesthetic? What advantages did it have over ether? What disadvantages did it have?
5. Describe the changes that have occurred for administering albuterol. Why have those changes occurred? What is albuterol used for?

6. Explain a medical function of ethyl chloride and Frigiderm and how they work.

7. Draw a structural formula and condensed formula of cyclopropane, cyclobutane, cyclopentane, and cyclohexane. In one of these molecules the C atoms are substantially non-planar. Which molecule is it? Draw and describe its actual shape. Which molecules are stable and which are not? Explain! What was the practical use for cyclopropane in the 1960s?

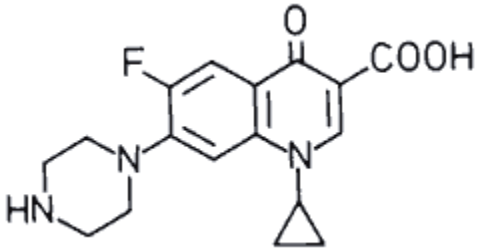
8. Draw all the structural and geometric isomers of a cyclopentane molecule in which two methyl groups are added to the ring. Give the

systematic names for each. Do the same for a cyclohexane molecule in which two ethyl groups are substituted on the ring.

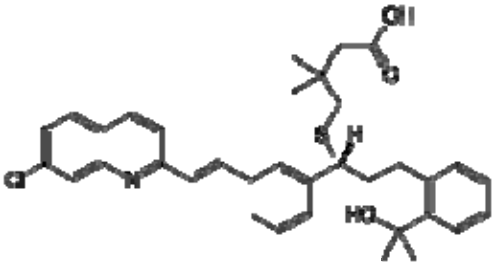
9. Draw the structure of the following molecules:

a) cis-1,3-dimethylcycloheptane b) trans-1,4 diethylcyclohexane c) cis-1-methyl-2-propylcyclohexane d) trans-1-chloro-3-iodocyclopentane

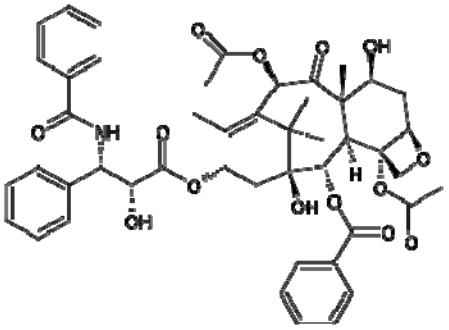
10.a) Label the functional groups in the molecule of ciprofloxacin (Cipro), an antibiotic. Which portion of the molecule would you expect to be particularly unstable based on bond angles?



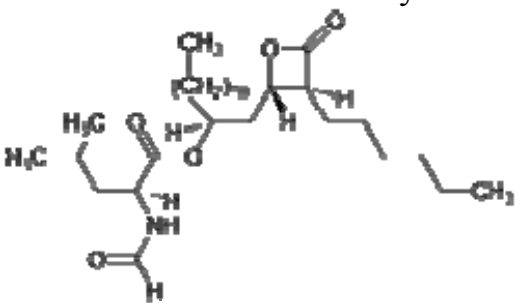
b) Label the functional groups in the molecule of montelukast (Singulair), a drug used in treatment of asthma. Which portion of the molecule would you expect to be particularly unstable based on principles learned in this unit and why?



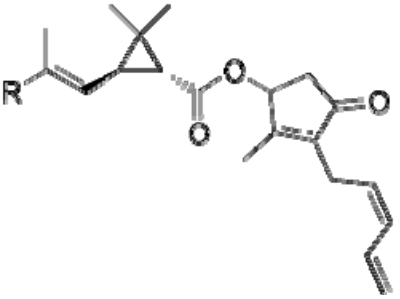
c) Label the functional groups in the molecule of paclitaxel (Taxol), an anticancer drug. Which portion of the molecule would you expect to be particularly unstable based on principles learned in this unit and why?



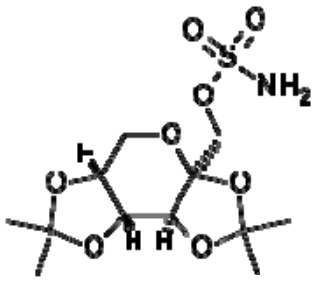
d) Label the functional groups in the molecule of orlistat (Xenical), an antiobesity drug which inhibits the formation of fat. Which portion of the molecule would you expect to be particularly unstable based on principles learned in this unit and why?



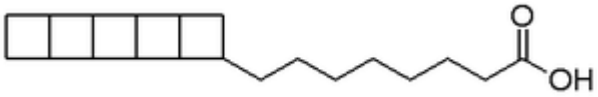
11. The structure of pyrethrin (an insecticide) is shown below. Identify the functional groups. The reactive group of pyrethrin is primarily due to one specific structure in the molecule. What is that group and why is it reactive?



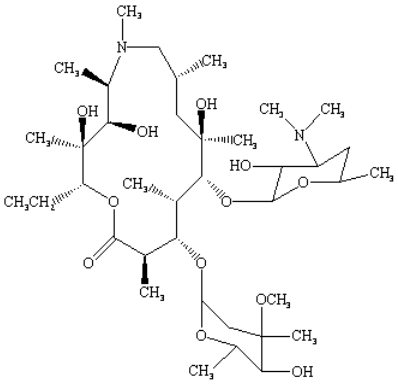
12. Topiramate(Topamax TM) is a drug marketed for treating seizures and migraine and is commonly prescribed (off-label) for many other conditions. Its structure is shown below. Identify the functional groups in topiramate. (The functional group with S is actually a sulfamate rather than a sulfonamide, because of the third O on the S; you don't have to remember that!) Give the bond angles in each ring and comment on the stability of each of those rings. What is the significance of the wedges and dashes?

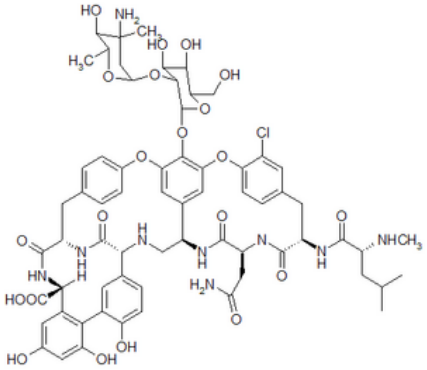


13. Some specialized bacteria have membranes which contain pentacycloanammoxic acid whose structure is shown below. Comment on the stability of this compound and explain your answer.



14. The structures of two common antibiotics are shown below.





Azithromycin(Zithromax) Vancomycin

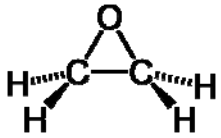
a) Identify the functional groups in each molecule

b) Explain the significance of the wedge and dash notations in the structures.

c) How many atoms are in the largest ring in each of azithromycin? Will it be stable or not? Explain your answer. Name the conformation of the 6-membered ring structures in these two antibiotics. Will the 6-membered rings be stable or not? Why?

Azithromycin(Zithromax) is a common antibiotic used to treat a wide variety of infections. Vancomycin is usually reserved for life threatening infections that are resistant to other antibiotics. It must be given IV and can occasionally cause anaphylactic shock and nephrotoxicity. What do we mean by nephrotoxicity and anaphylactic shock?

15. Ethylene oxide has been used as a chemical sterilizer for medical instruments that cannot withstand the high temperatures of an autoclave. What are the bond angles in ethylene oxide? Comment on its stability.



16. What is the technical term for an atom which has 4 different groups bonded to it?

17. How are molecules with a chiral center different from molecules which do not have a chiral center? Draw a one-carbon molecule with a chiral center.

18. What is the term for mirror image molecules which are not identical ("superimposable"). Draw an example of two one-carbon molecules which are enantiomers.

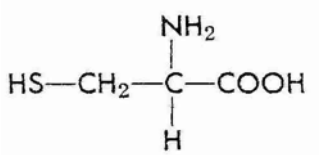
19. Give the newer terms for asymmetric C; optical isomer.

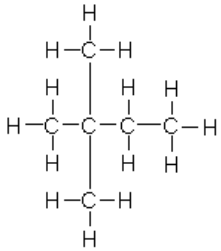
20. What sort of light is used to differentiate between two enantiomers? Explain how it is used.

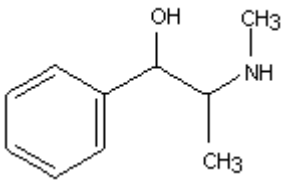
21. Give 3 pairs of prefixes that are used to differentiate between pairs of enantiomers.

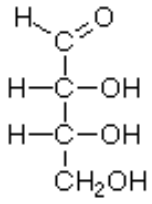
22. Explain why enantiomeric drugs usually have only one form that actually has high activity. Give two examples of drugs that are racemic mixtures. Define the term racemic mixture.

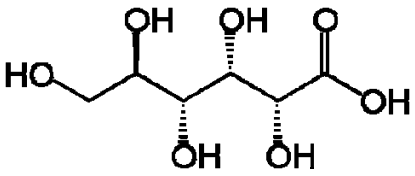
23. Label any chiral centers in the molecules below with an *.

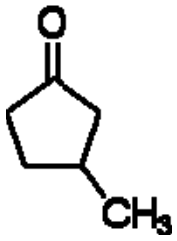






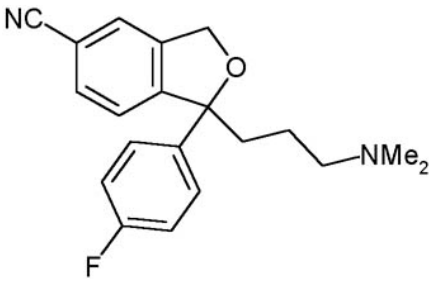






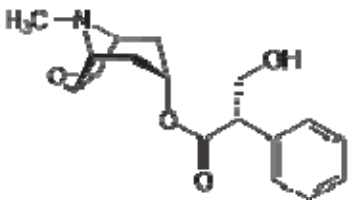
3-methylcyclopentanone 4-methylcyclohexanone

24.Citalopram (Celexa) is a commonly used antidepressant whose structure is shown below. Label the functional groups and label any chiral atoms. (Me stands for a methyl group.) Citalopram is actually a racemic mixture.

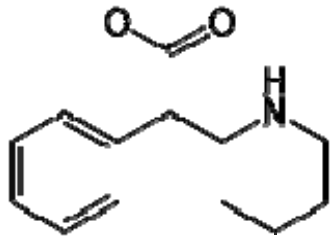


Like other drugs mentioned in the text the pure active enantiomer has been marketed. Its generic name is escitalopram or Lexapro. Compare the generic names of the racemic mixture and the pure enantiomer and explain the origin of the prefix in front of the generic name.

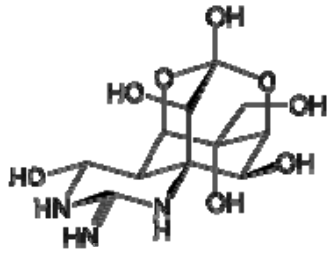
25. Scopolamine is commonly used as a patch behind the ear to reduce motion sickness. Its structure is shown below. Identify the functional groups and chiral centers in the molecule. How many members are in each ring?



26. Identify functional groups and label chiral centers in methylphenidate (Ritalin)



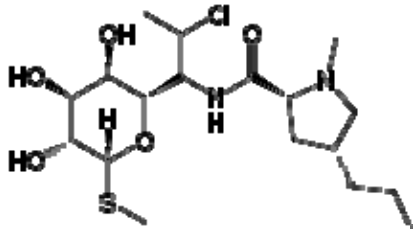
27. The structure of tetrodotoxin is a very potent neurotoxin that blocks sodium channels in cell membranes. It is found in pufferfish, western newts, blue-ringed octopi and some other organisms. Identify the functional groups in the molecule and indicate the bond angles in each of the rings.



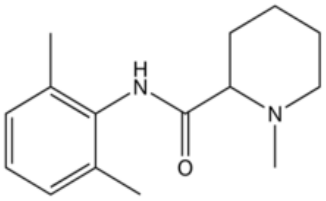
Tetrodotoxin

28. Discuss fen-phen in terms of enantiomers. Do the same for epinephrine, albuterol and Prilosec. Which of the previous molecules is marketed as a pure enantiomer?

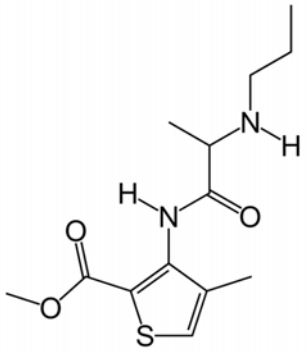
29. a) The structure of the antibiotic clindamycin is shown below. Label the functional groups and indicate chiral centers with a *.



b) Label the functional groups and chiral centers in mepivicaine, a local anesthetic.



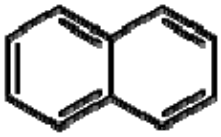
c) Label the functional groups and chiral centers in the molecule below



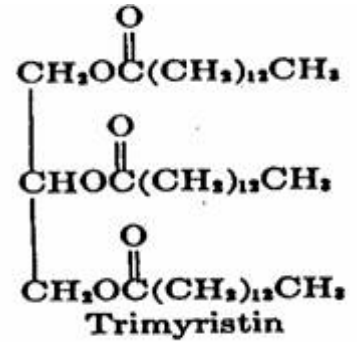
30. Discuss the solubility of alkanes in water. What happens if an OH or other polar group is substituted on an alkane chain? How long a non-polar alkane chain can be pulled into water solution by an OH group? How long a non-polar alkane chain can be pulled into water solution by an ionic group such as carboxylate or ammonium ion?

31. Predict the solubility in water of the following molecules:
a) cyclohexane

b) naphthalene =



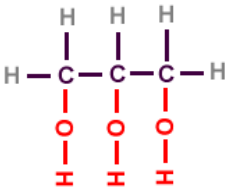
c) trimyristin =



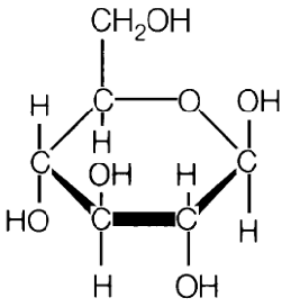
Trimyristin

d) glycerin

e) dextrose



Glycerol
propane1,2,3 triol



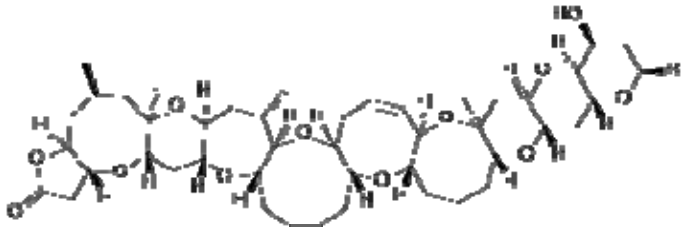
32. What purification technique is used to separate petroleum into the various products (gasoline, diesel, lubricating oil)?

33. How do gasoline, diesel and lubricating oil differ in terms of a) length of C chain and b) qualitative boiling point?

34. Give two health uses of mineral oil.

35. How does petrolatum differ from mineral oil in terms of length of chain and physical properties? Name several consumer products made of petrolatum.

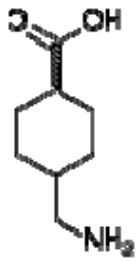
Brevetoxin is another potent sodium channel blocking neurotoxin that is made by a phytoplankton called Karenia brevis, most commonly in the eastern Gulf of Mexico. It is responsible for the "red tides" (an algal overbloom) that occurs on a regular basis. As you can see from the structure below, mother nature likes rings. Identify all the functional groups.



What is the significance of the wedges and dashes?
A variety of different types of plankton making different toxins can cause "red tides". There is speculation that Exodus 7:17-18 is probably describing such an event:

"Behold, I will smite with the rod that is in mine hand upon the waters which are in the river, and they shall be turned to blood. And the fish that is in the river shall die, and river shall stink and the Egyptians shall be loathe to drink of the water of the river."

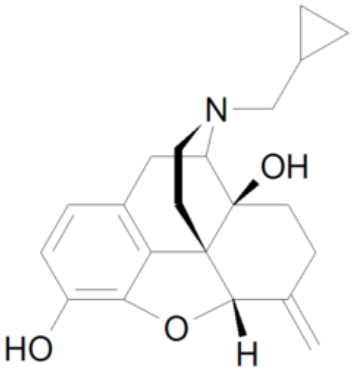
Draw the structure of tranexamic acid(Cyklokapron) showing the real conformation of the ring.



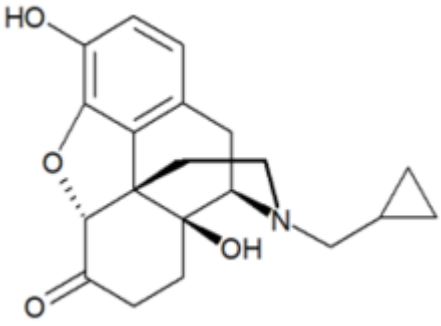
Using Google, what is tranexamic acid used for?

Chiral centers of 3 methyl-3-hydroxycyclobutanone glucuronic acid rhamnose

ribulose



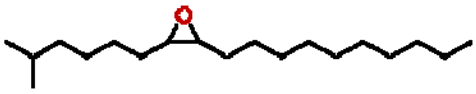
Nalmefene



Naltrexone

www.matrixlabsindia.com/inside/antihistamine.asp

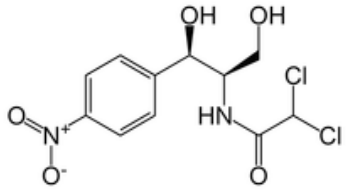
Deltaamethrin(popular insecticide)



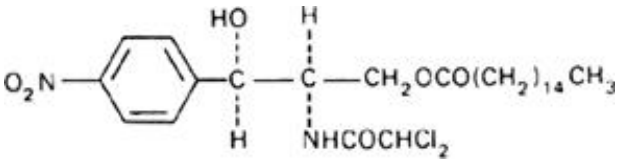
dispalure (gypsy moth attractant)

What reactive groups are found in the above molecules?

f) chloramphenicol



chloramphenicol palmitate



15. Draw an ammonia molecule (NH_3). Label which atoms on the NH_3 molecule have partial positive and negative charges. Will ammonia be soluble in water? Show how water molecules will arrange themselves around an ammonia molecule to maximize attractions. What is the specific name for those attractions?

2-methylcyclopentanone 2-methylcyclobutanol **Digging deeper**.

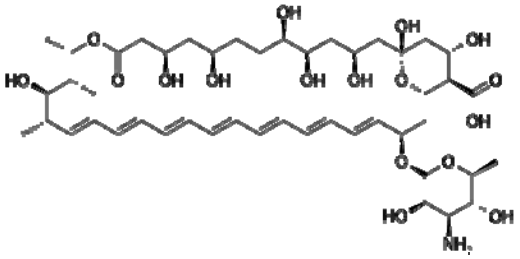
Obtain a spray can (e.g. hair spray) and see if you can guess which of the inert ingredients is being used as the propellant (the molecule under pressure that forces the spray out

Do an internet search on halons and write a brief paper (1-2 pages, double spaced) on what their chemical structures are, their practical uses, and why their use has been phased out. Cite your references.

16. Do the same for bromomethane (methyl bromide).

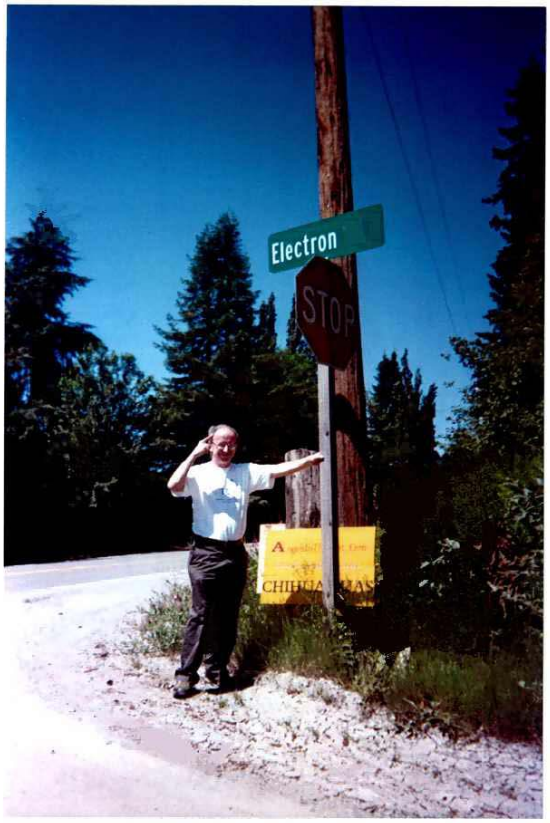
17. A 2007 proposal has suggested that bromomethane (methyl bromide) be replaced with iodomethane (methyl iodide). This proposal has been met with widespread opposition from a large contingent of scientists. Do a Google search and summarize some of the reasons why there are major concerns about using methyl iodide.

The structure of the anti-fungal drug amphoteracin-B is shown below. It is thought to work in a manner similar to Nystatin and natamycin. What is that mechanism and what portion of the structure is thought to play a role in that mechanism.



Amphoteracin-B

Digging deeper, Crown ethers, see Journal of Inclusion Phenomena 6: 337-350, 1988


Electron
STOP