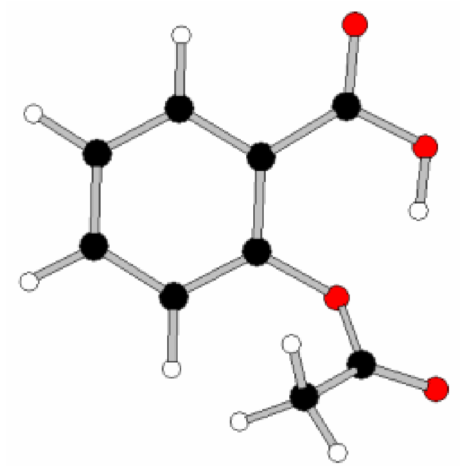

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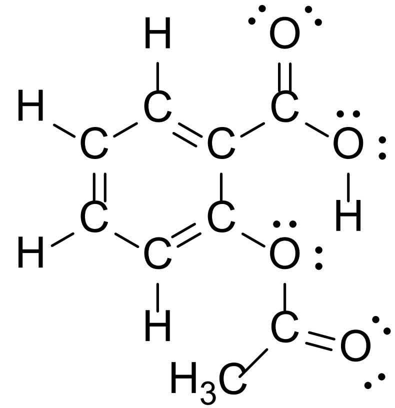

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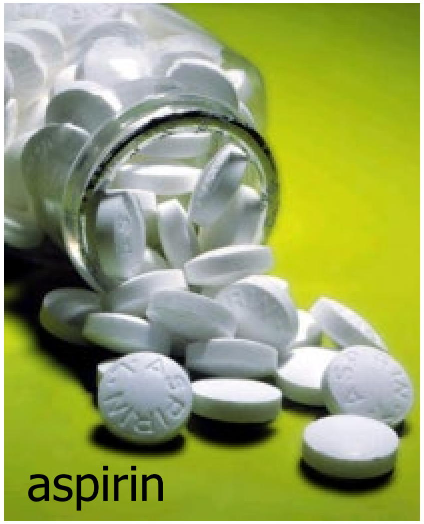


CHEMISTRY 2000

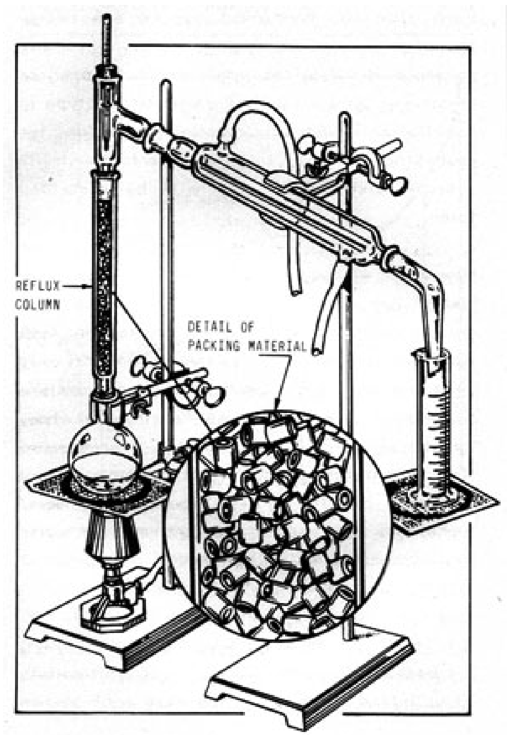
Topic #3: Organic Chemistry

Fall 2020

Dr. Susan Findlay

See Exercises 10.1 to 10.5

→



What is Organic Chemistry?

- Originally, organic chemistry was the study of molecules that came from organic (i.e. alive at some point) sources. Since then, the field has expanded to include the study and preparation of molecules that don't occur naturally but are similar in structure to molecules that do occur naturally:
  - Penicillin and streptomycin are naturally occurring antibiotics, so they fit under the original definition of organic molecules.
  - Ampicillin is a semisynthetic antibiotic whose structure is essentially a modified penicillin; it's still considered to be an organic molecule.
  - Sulfonamides ("sulfa drugs") are completely synthetic antibiotics, but they're also considered to be organic molecules.
- What's the common thread that ties these molecules together?

CARBON

- Organic chemistry is the study of carbon-containing molecules that aren't minerals. *(CO_2, $CaCO_3$ and $NaHCO_3$ contain carbon but aren't considered to be organic.)*

What is Organic Chemistry?

- What do organic chemists do? Depends. There are a number of subdisciplines, but here are a couple of examples:
  - Drug design
    - Most pharmaceutical companies have research departments where some chemists use computers to model what shape/polarity a drug needs to be in order to get to and bind to a target site.
    - Other chemists work out how to make molecules that will have this shape/polarity, often designing new reactions in the process.
    - Finally, if a molecule is made that has both the desired activity <u>and</u> is safe, another group of chemists designs a series of reactions that can make the potential drug in a safe manner on a large scale (using really cool really *BIG* equipment!)
  - Structural determination
    - When a plant/marine/etc. extract is found to have interesting properties, a chemist separates out the different molecules in the extract and uses modern equipment to help them determine the structures of the molecules involved – a lot like solving puzzles. These chemists get to go on great field trips!

What is Organic Chemistry?

- Energy-related research
  - Petroleum products are organic molecules. So are biofuels.
- Environmental and agricultural sciences
  - Design of newer, better, (hopefully) safer herbicides and pesticides is done by chemists.
  - Chemists are also involved in environmental remediation – designing methods to try and remove (or at least detoxify) chemicals from the environment.
- Basic research
  - In every field of science, there are some scientists who do research just for the sake of learning. Because they're not driven by any particular agenda, they often produce ideas that lead to completely new understanding of our world – and sometimes technology nobody had imagined before.
- Education
  - Obviously. I'm here, aren't I? ☺

Drawing Organic Molecules

- Carbon is the backbone of any organic molecule – literally.
  - A neutral carbon atom has 4 bonds and 0 lone pairs.
  - A carbon atom can have tetrahedral, trigonal planar or linear molecular geometry:
  - Carbon DOES NOT* have 90° angles!!! For this reason, I will draw organic molecules in a zig-zag fashion:
  - Because carbon needs to form 4 bonds in order to be neutral and obey the octet rule, it is capable of forming a wide variety of chains and rings. More than 7 billion organic compounds are currently known and over a million new ones are discovered every year!

*unless forced to by being in a 4-atom ring

Drawing Organic Molecules

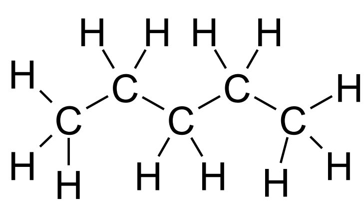
- It is important for chemists to know which atoms are connected to which other atoms. It is not enough to write C_2H_6O. We must show how the atoms are connected:

- The structures above are **structural formulas**. They show the location of every atom in the molecule. For very large molecules, structural formulas take a long time to draw and can be confusing to read. Because of this, chemists have developed other methods for drawing structures.
- In a **condensed structural formula**, we group hydrogen atoms with the atoms they're attached to and leave out the single bonds:

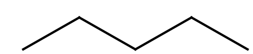
Drawing Organic Molecules

- In a **line-bond structure**, we do not draw the hydrogen atoms attached to carbon. We also replace each 'C' with a dot and connect the dots with lines (i.e. each line is a bond)

- **If you write the 'C', you <u>must</u> write <u>all</u> the atoms bonded to it as well:**

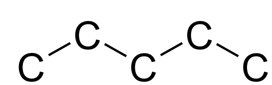


or $CH_3CH_2CH_2CH_2CH_3$ *or*



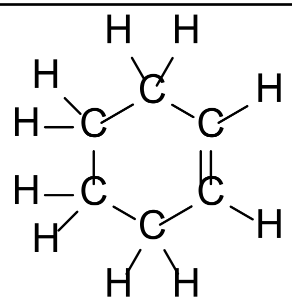
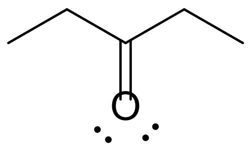
(structural formula) *(condensed structural formula)* *(line-bond structure)*

NOT



Drawing Organic Molecules

- Complete the table and write each molecular formula at the left

Structural Formula	**Condensed Structural Formula**	**Line-Bond Structure**
		
	$H_2C{=}CHCH_2Cl$	
		

Functional Groups

- Organic compounds are often classified based on the functional groups they contain because functional groups play a key role in determining a compound's physical and chemical properties.

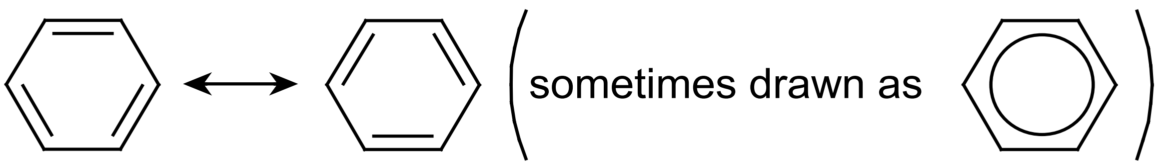
- A functional group is part of an organic molecule that contains:
  - a **heteroatom** (atom other than C or H; usually N, O or S) and/or
  - a **multiple bond** (double or triple)

- So, essentially what we're looking for are:
  - polar bonds
  - lone pairs
  - π bonds

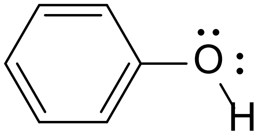
  which makes sense since these are the reactive parts of organic molecules. *Note that this makes alkanes "organic compounds without functional groups" since they contain only C-H and C-C single bonds.*

Functional Groups

- Functional groups with carbon-carbon multiple bonds:
  - Alkene (contains C=C)
  - Alkyne (contains C≡C)
  - Arene (contains 6 atoms in a ring with 3 π bonds):*



- Functional groups with single bonds to N, O or S:
  - Amine (contains C–N)
  - Ether (contains C–O–C)
  - Alcohol (contains C–O–H)
  - Phenol (contains C–O–H where C is part of an arene):

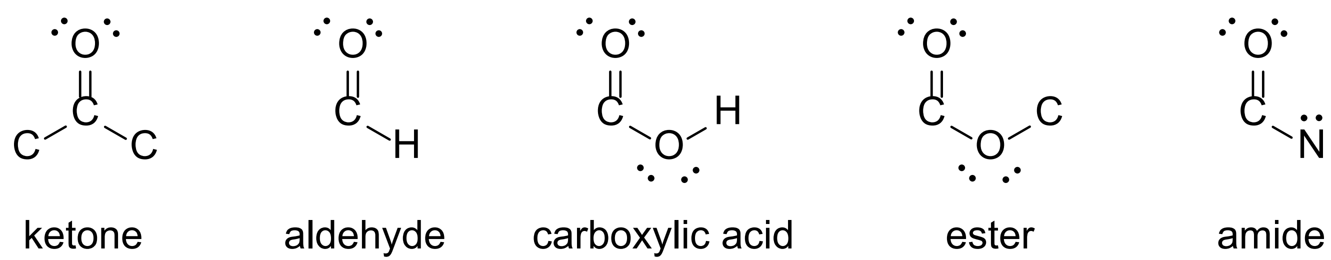


  - Thiol (contains C–S–H)

*This definition expands if you take further courses in organic chemistry.

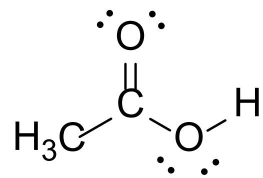
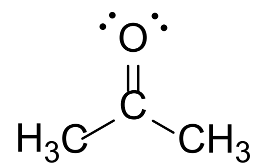
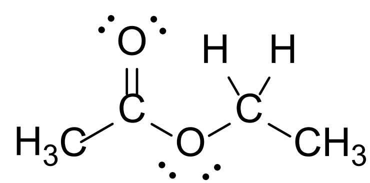
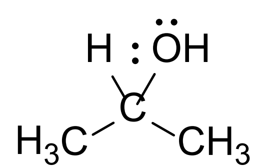
Functional Groups

- Functional groups with multiple bonds to N, O or S:
  - Ketone (contains C=O with two C attached)
  - Aldehyde (contains C=O with H attached)
  - Carboxylic Acid (contains C=O with OH attached)
  - Ester (contains C=O with O–C attached)
  - Amide (contains C=O with N attached)
  - Nitrile (contains C≡N)

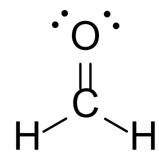
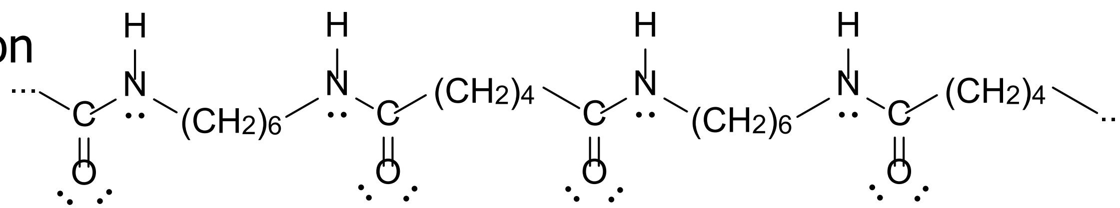
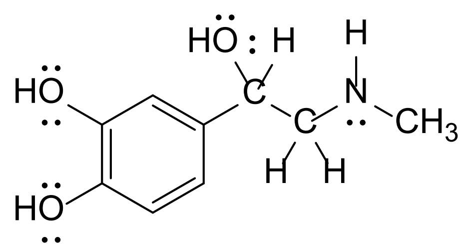
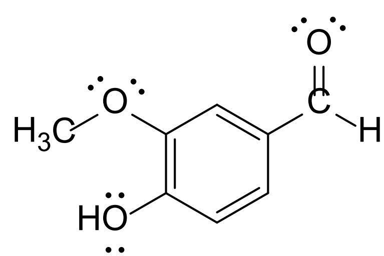


- Because it's an important part of so many functional groups, **C=O** has a special name. It's called a **carbonyl**.
- Similarly, the term **hydroxy** is often used to describe just the **–OH** part of an alcohol and **carboxy** refers to the **CO_2** part of an ester or carboxylic acid.

Functional Groups

Compound	Structure	Functional Group(s)
Acetic acid (vinegar)		
Acetone (nail polish remover)		
Ethyl acetate (acetone-free nail polish remover)		
Isopropanol (rubbing alcohol)		

Functional Groups

Compound	Structure	Functional Group(s)
Formaldehyde (biology labs)		
Nylon		
Adrenaline (Epinephrine)		
Vanilla extract (Vanillin)		

Isomers

- Shape is crucial in organic chemistry. A molecule’s shape helps to determine how it interacts with other molecules because it determines which atoms are able to come close enough together in space to interact.

- **Isomers are compounds that have the same molecular formula but different arrangements of atoms.**

- Isomers can only exist as pairs or groups. Just as you cannot be a sibling without having a sibling, a molecule cannot be an isomer without having an isomer.

Isomers

- Isomers can be divided into two main categories:
  - **Structural isomers** have **different connectivity**.
    In other words, there will be a difference in which atoms are connected to which:
  - **Stereoisomers** have the **same connectivity** but different shapes. We saw examples of stereoisomers when we looked at *cis-* and *trans-* complexes in the co-ordination chemistry section of CHEM 1000:

Structural Isomers

- Structural isomers have different physical properties from each other (melting point, boiling point, etc.). This is also the only kind of isomerism for which the different isomers can have different functional groups.

  e.g. C_3H_8O has three structural isomers:

When drawing isomers, all structures must be valid Lewis diagrams!
Avoid drawing atoms with non-zero formal charges or that don't obey the octet rule.

Structural Isomers

- A molecule's "unsaturation index" refers to the total number of rings plus pi bonds. It will be the same for all isomers. It can either be calculated using the formula $UI = \frac{2C+2+N-X-H}{2}$ or read directly off the Lewis diagram for one valid isomer.

- What is the unsaturation index for C_3H_6?

- Draw all structural isomers for C_3H_6.

Structural Isomers

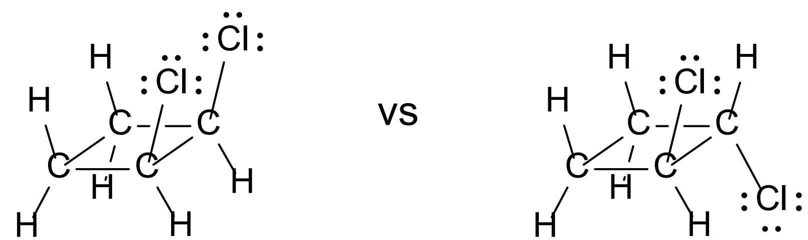
- Draw all structural isomers for C_6H_{14}.

Structural Isomers

- Draw all structural isomers for C_3H_9N.

Stereoisomers: Geometric Isomers

- **Geometric isomers** are stereoisomers which differ based on whether groups are on the same side or opposite sides of a ring or double bond:

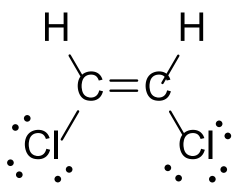


- The isomer with the two more important* groups on the same side of the ring/double bond is called the ***cis-*** isomer while the isomer with the two more important groups on opposite sides of the ring/double bond is called the ***trans-*** isomer.

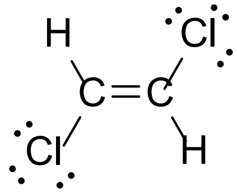
* The importance of a group is determined by the mass of the first atom. So, Cl is more important than CH_3 which is, in turn, more important than H.

Stereoisomers: Geometric Isomers

- Geometric isomers have different physical and chemical properties. Of the geometric isomers shown below, which would you expect to have a higher boiling point?

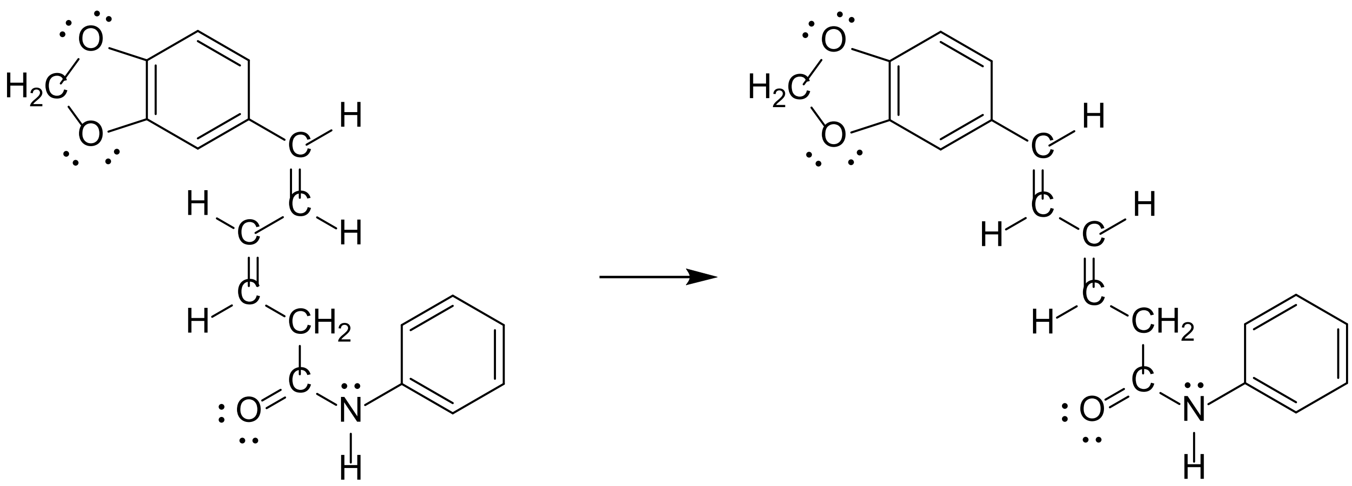


vs



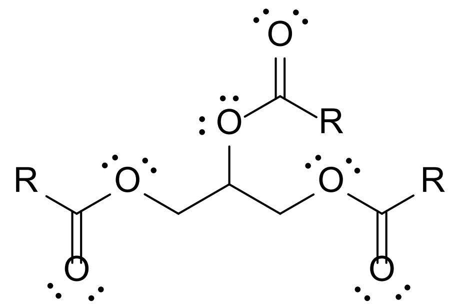
Stereoisomers: Geometric Isomers

- Chavicine is the molecule responsible for the flavour and smell of black pepper. In the peppercorn, it exists as the *cis,cis*-isomer. After it is ground, it is slowly converted to the *trans,trans*-isomer which has less flavour and aroma:

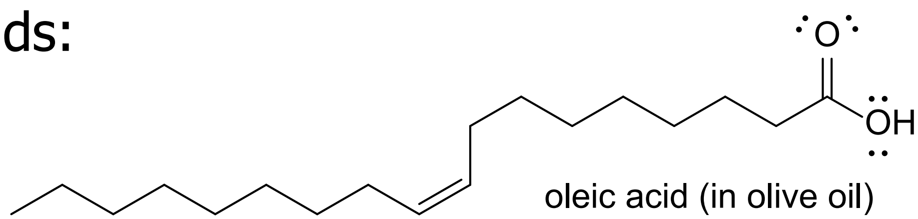


Stereoisomers: Geometric Isomers

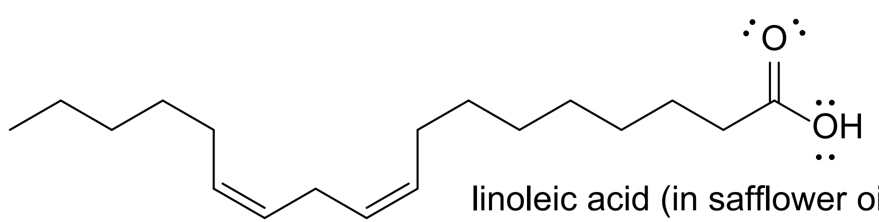
- Unsaturated fats contain *cis* double bonds. Each fat contains three fatty acids ($R\text{-}CO_2H$) attached to a glycerol residue:



- Monounsaturated fats have fatty acids with one *cis-* double bond while polyunsaturated fats have fatty acids with several *cis-* double bonds:



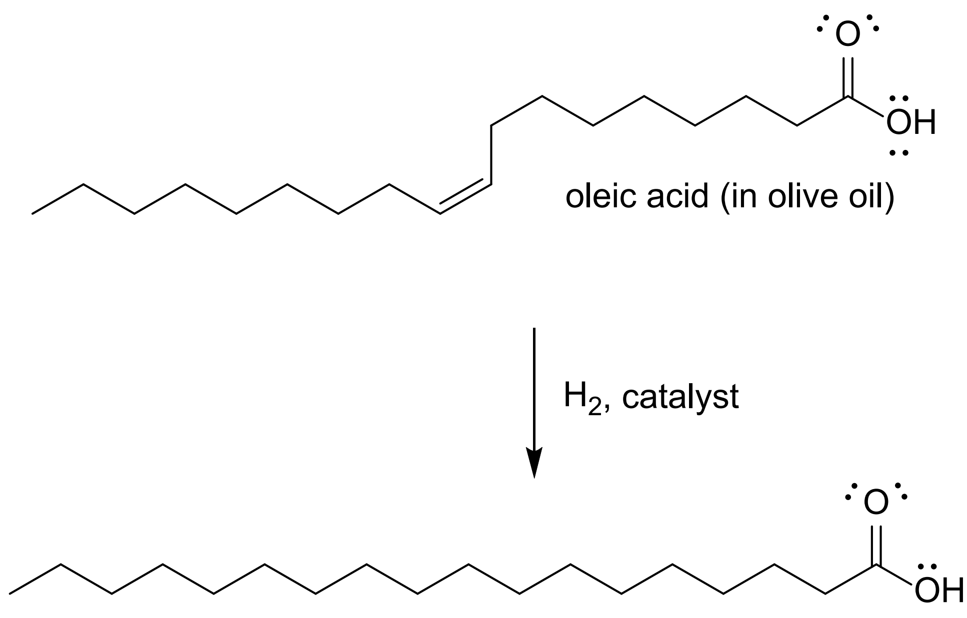
oleic acid (in olive oil)



linoleic acid (in safflower oil)

Stereoisomers: Geometric Isomers

- Our bodies need fats containing *cis-* double bonds; however, these fats tend to exist as liquids. To make solid fats (like margarine), a process called hydrogenation is used to 'saturate' the fats with hydrogen:

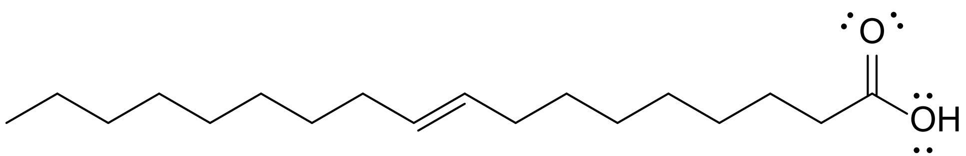


stearic acid (a saturated fatty acid)

Stereoisomers: Geometric Isomers

- Saturated fats pack together more readily than fats containing *cis*-double bonds, so they can clog arteries and cause other health problems when consumed in excess.

- Worse yet are *trans*-fats which contain fatty acids with unnatural *trans*-double bonds which also pack together easily <u>and</u> which the body doesn't have the enzymes to break down properly:

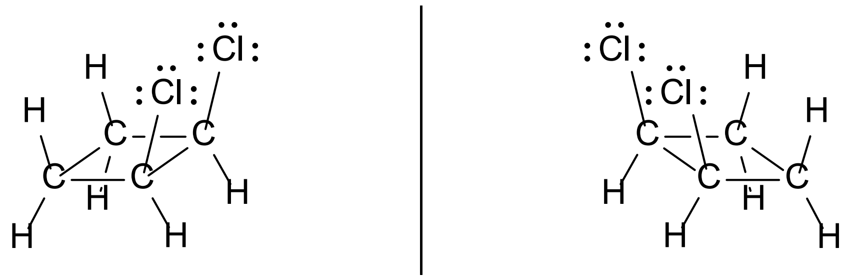


a trans fatty acid

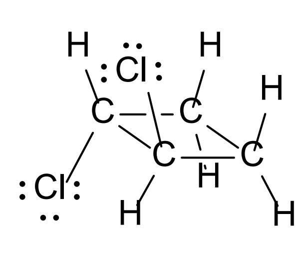
- *Trans-* fatty acids are a by-product of partial hydrogenation. The conditions used to add hydrogen across some of the natural double bonds allow the remaining double bonds to isomerize.

Stereoisomers: Enantiomers and Chirality

- **Enantiomers** are stereoisomers which are mirror images of each other.
  - The two molecules below are mirror images of each other, but one can be turned around and superimposed on the other. They are not enantiomers. They are the same molecule.

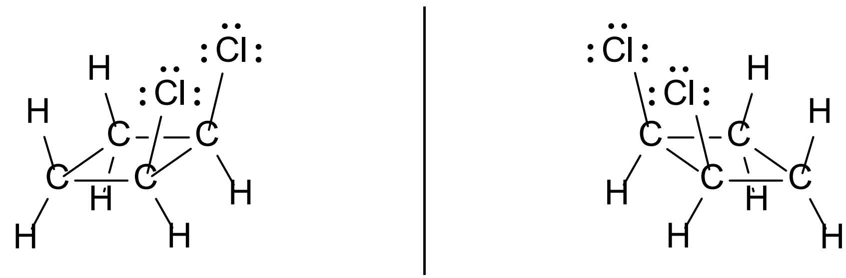


  - The two molecules below are mirror images of each other. No matter how we turn either molecule around, they cannot be superimposed. They are enantiomers!

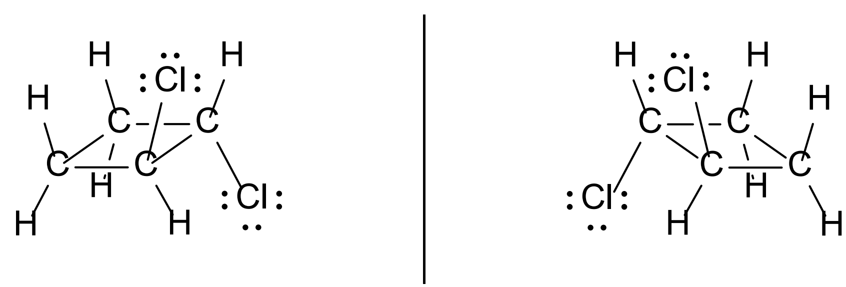


Stereoisomers: Enantiomers and Chirality

- Any molecule which does not have an enantiomer (because it is superimposable with its mirror image) is termed **achiral**.

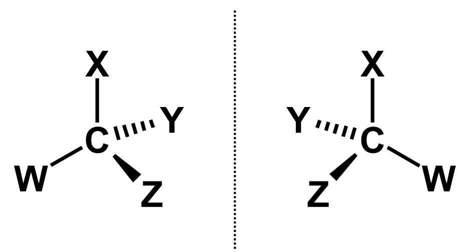


- Any molecule which has an enantiomer is termed **chiral**. An old fashioned synonym for the term "chiral" is "optically active" which refers to the fact that chiral molecules rotate plane-polarized light (light in which the waves are all parallel).



Stereoisomers: Enantiomers and Chirality

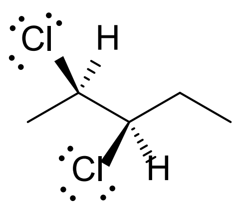
- Most chiral molecules contain one or more **chirality centers**. In organic chemistry, a chirality center is usually a tetrahedral atom with 4 different groups attached:



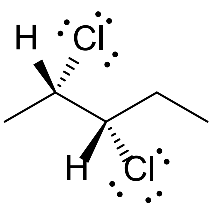
- Be aware that some achiral molecules also contain two or more chirality centers, so you are better off looking at the relationship between the molecule and its mirror image. For this reason, organic chemists are very fond of their molecular model kits! (*available from either the university bookstore or the CBC club; if you plan to take CHEM 2500 and want to pass, you will be buying one for that course, so may as well get one now…)*

Stereoisomers: Enantiomers and Chirality

- The standard way to draw chiral molecules is to use line-bond structures with wedges and dashes to show stereochemistry:
  - The longest chain is drawn as a zigzag in the plane of the page.
  - Wedges are used for groups pointing out of the page at you.
  - Dashed lines are used for groups pointing away from you.
  - It's best to draw all four groups attached to each chirality centre.



and

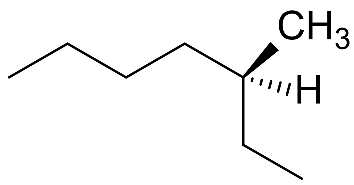


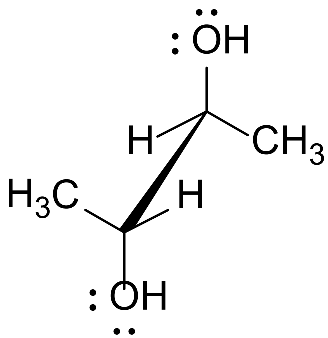
are enantiomers

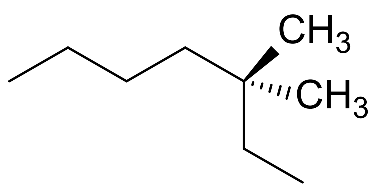
- Show two more ways to draw the mirror image of the molecule on the left.

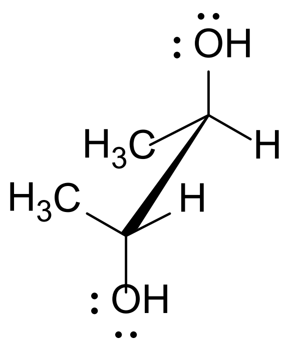
Stereoisomers: Enantiomers and Chirality

e.g. For each of the following molecules, locate the chirality center(s) and decide whether the molecule is chiral or achiral.









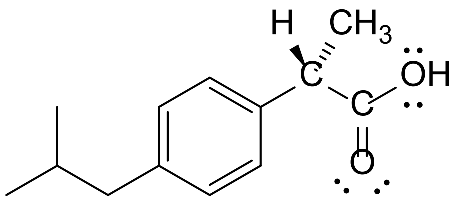
Stereoisomers: Enantiomers and Chirality

- Unlike other kinds of stereoisomers, the physical and chemical properties of a pair of enantiomers are identical unless they are in a chiral environment (such as any biological system).

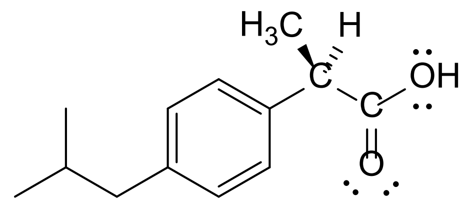
- Your hands are chiral and can be used as an analogy for enantiomers - left and right hands are mirror images that cannot be superimposed. If you have a right-hand glove, it will not fit properly on your left hand (and vice versa). Similarly, because enantiomers have different shapes, one enantiomer of a hormone may fit nicely into a pocket in a protein, but the opposite enantiomer won't. That means that the opposite enantiomer of hormone won't do its job. In this case, the 'wrong' enantiomer of hormone is useless, and it would be a waste of energy for the body to make it.

Stereoisomers: Enantiomers and Chirality

- Many drugs are chiral and act in the same way. Ibuprofen is sold as a mixture of enantiomers, but only one is active.



active



inactive

- Find the chirality center in each enantiomer of ibuprofen.

Stereoisomers: Enantiomers and Chirality

- Sometimes, the 'wrong' enantiomer is not just a waste of energy. It might fit into a different pocket in the protein (or another protein) or bind too strongly/weakly, giving a completely different effect than the 'right' enantiomer.

- One of the most famous and tragic examples of this effect was the drug Thalidomide which was prescribed as a medication for morning sickness in the late 1950s and early 1960s. One enantiomer of this drug was effective in combating morning sickness; however, the other enantiomer caused severe birth defects in the children of the women who took it. It was pulled from the market 4 years after its release, but not before many 'Thalidomide babies' had been born.

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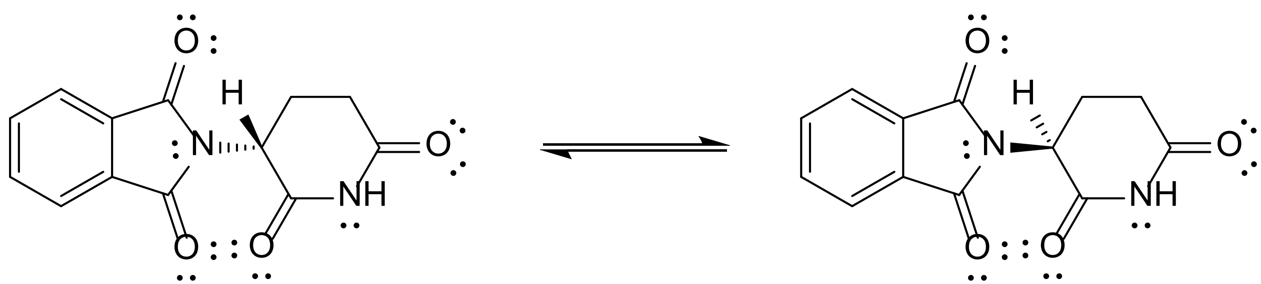
- To make matters worse, the two enantiomers of thalidomide are interconverted within the human body so it's impossible to prescribe only the "good" enantiomer:



sedative

teratogenic (causes birth defects)

- Since this tragedy, there have been much tighter regulations on testing of chiral drugs. For any drug that can be converted to the other enantiomer within the body, both enantiomers must be tested as well as a mixture.