Objective 12

Apply VSEPR Theory to determine shape Identify polar bonds from electronegativity Determine polarity of molecule from shape Determine intermolecular forces from polarity

Intro to Organic Compounds
Draw skeletal structures
Intro to Biochemistry

Structure ---> Shape ---> Properties, e.g., Polarity Water is the Universal Solvent What Makes a Substance Soluble in Water?

Draw the structure of water.

The shape of water is:

- a) tetrahedral
- b) trigonal planar
- c) linear
- d) trigonal pyramid
- e) bent

Water is:

f) Polar

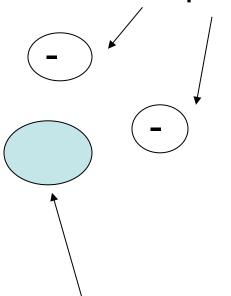
g) non-polar

Is HCl soluble in water? Yes No Give reasons for your answer.

Molecular Structure Determines Shape Which Determines Properties

Shape is determined from *Valence Shell Electron Pair Repulsion* (VSEPR) Theory

Electron pair



Central atom

Like charges *repel*.

Where should the electron pairs be located so they are as far away from each other as possible?

Shape depends on # of e- pairs around the central atom

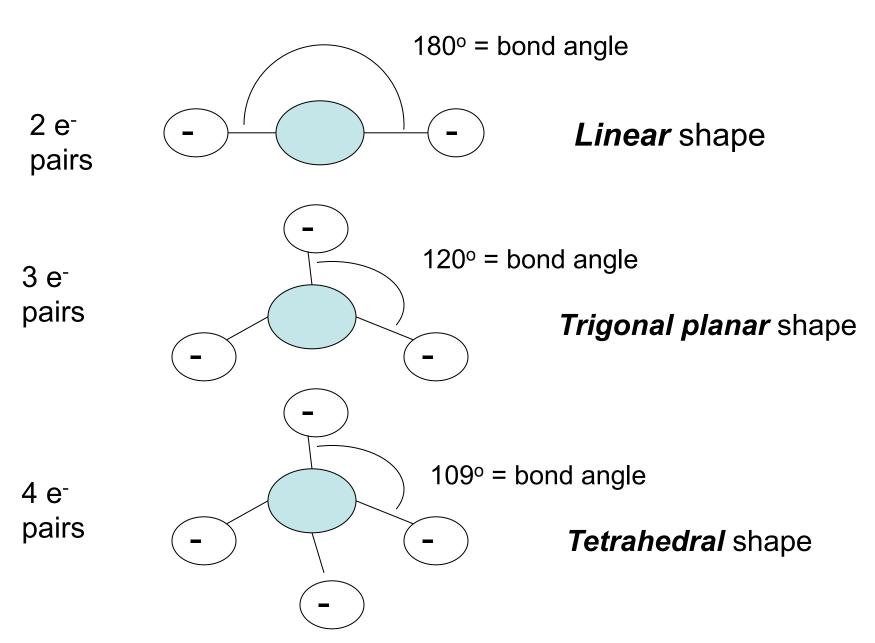


Table 1. Shape at a *Central Atom* Based on VSEPR Theory

# of e ⁻ pairs	# of bonding pairs	# of lone pairs	Shape	Example
2	2	0	Linear	BeH ₂
3	3	0	Trigonal planar	BH ₃
4	4	0	Tetrahedral	CH ₄
4	3	1	Trigonal pyramid	NH ₃
4	2	2	Bent	H ₂ O

of e⁻ pairs = # of bonding pairs + # of lone pairs

VSEPR Theory Tells You the <u>Shape at Each Central</u> <u>Atom</u>

Treat a **Double** Bond or **Triple** Bond the **Same** as a **Single** Bond.

E.g., ethylene = C_2H_4 .

Draw the Lewis structure.

At C, two single bonds and one double bond.

Treat <u>double bond like a single bond</u> ==> so <u>C has three</u> <u>bonding pairs</u> ==> Shape is <u>trigonal planar</u> at C.

Acetone = $(CH_3)_2CO$ Draw the Lewis structure. What is the shape at each C?

Electronegativity Determines Bond Polarity Bond Polarity and Shape Determines Polarity of Molecule

Electronegativity (EN) is the ability of an atom in a bond to attract electrons toward itself.

Bond between <u>Same</u> atoms ==> EN is the <u>Same</u> ==> equal sharing of the bonding pair of electrons ==> <u>non-polar bond</u>

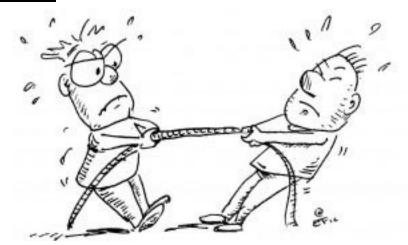
Bond between <u>Different</u> atoms ==> EN is <u>Different</u> ==> unequal sharing of the bonding pair of electrons ==> <u>polar</u> bond

Electronegativity Determines Bond Polarity

<u>Electronegativity</u> (EN) is the ability of an atom in a bond to attract electrons toward itself.

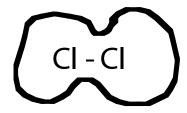
Tug of War for electrons in a bond ==> the more EN atom

wins!



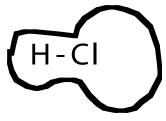
http://biggirlbombshell.com/index.php/ 2012/06/tug-of-war/

Compare non-polar CI-CI to



Uniform e⁻ density no (+) or (-) pole

polar H-Cl.



Non-uniform e⁻ density H is (+) pole, Cl is (-) pole

Structure ---> Shape ---> Properties, e.g., Polarity

Water is the Universal Solvent What Makes a Substance Soluble in Water?

"Like Dissolves Like"

Draw the structure of water.

The shape of water is:

- a) tetrahedral
- b) trigonal planar
- c) linear
- d) trigonal pyramid
- e) bent

Water is:

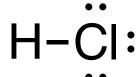
f) Polar g) non-polar

HCI is soluble in water. HCI and water are both polar.

H, 0, H

bent

polar



linear polar

Shape Determines Polarity of Molecule Polarity Determines Solubility

"Like Dissolves Like" (Solubility):

<u>polar</u> substances are <u>soluble</u> in <u>polar</u> solvents <u>non-polar</u> substances are <u>soluble</u> in <u>non-polar</u> solvents.

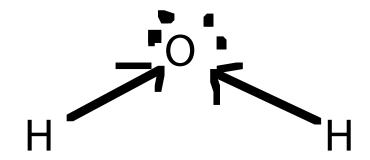
Is water polar or non-polar?

- (i) Draw Lewis structure.
- (ii) Determine shape using VSEPR theory.
- (iii) Is O-H bond polar? If so, draw an arrow toward the more EN atom.
- (iv) Each H pushes on O. Does O move?

 If yes ==> polar

 If no ==> non-polar

Water is polar!



Rubbing Alcohol (C₃H₈O) is used as a solvent and disinfectant.

Which structure is rubbing alcohol?



http://
www.drugfreeh
omes.org/
2013/05/whydrinkingrubbingalcohol-isharmful.html

Rubbing Alcohol (C₃H₈O) is used as a solvent and disinfectant.

Which structure is rubbing alcohol?

C

What is the shape at the C bonded to the O? What is the shape at the O? Is rubbing alcohol polar or non-polar? What is the dipole moment of rubbing alcohol? Is rubbing alcohol soluble in water?

What does Polarity have to do with Dipole Moment?

Polar Molecule means Dipole Moment ≠ 0

Non-Polar Molecule means Dipole Moment = 0

Substance	Dipole Moment, D
CO ₂	0
HCI	1.08
NH ₃	1.42
H ₂ O	1.85
CH ₂ O (formaldehyde)	2.2

Which compound is the most polar?

Polarity Determines Solubility in Water

Methane burns in air to produce carbon dioxide and water.

- a. Draw the Lewis structures of each reactant and product.
- b. Determine the shape of each substance.
- c. Determine the polarity of each substance.
- d. Which substance is soluble in water?

Salt, NaCl, is soluble in water. Explain why.

Ammonia, NH₃, is a gas at room temperature. It is bubbled through water to make aqueous ammonia (ammonium hydroxide). Explain why ammonia is soluble in water.

Ethanol, C₂H₅OH, is the alcohol in adult beverages and is a common organic solvent. Is ethanol soluble in water? Give reasons.

Top 10 Chemicals in the U.S. (2000)

2000 RANK	CHEMICAL	2000 PRODUCTION (in 10 ⁹ kg)	FORMULA
(by mass)			
1	Sulfuric acid	39.62	
2	Ethylene	25.15	C_2H_4
3	Lime	20.12	
4	Phosphoric acid	16.16	
5	Ammonia	15.03	NH_3
6	Propylene	14.45	C_3H_6
7	Chlorine	12.01	
8	Sodium hydroxide	10.99	
9	Sodium carbonate	10.21	
10	Ethylene chloride	9.92	C ₂ H ₄ Cl ₂

Which of the Top 10 Chemicals are organic compounds?

Organic (Carbon-Containing) Chemistry is the Biggest, Most Studied Field of Chemistry

There are a **lot** of organic compounds = 16 million known in the world (

http://wiki.answers.com/Q/How many organic compounds are known in the world)

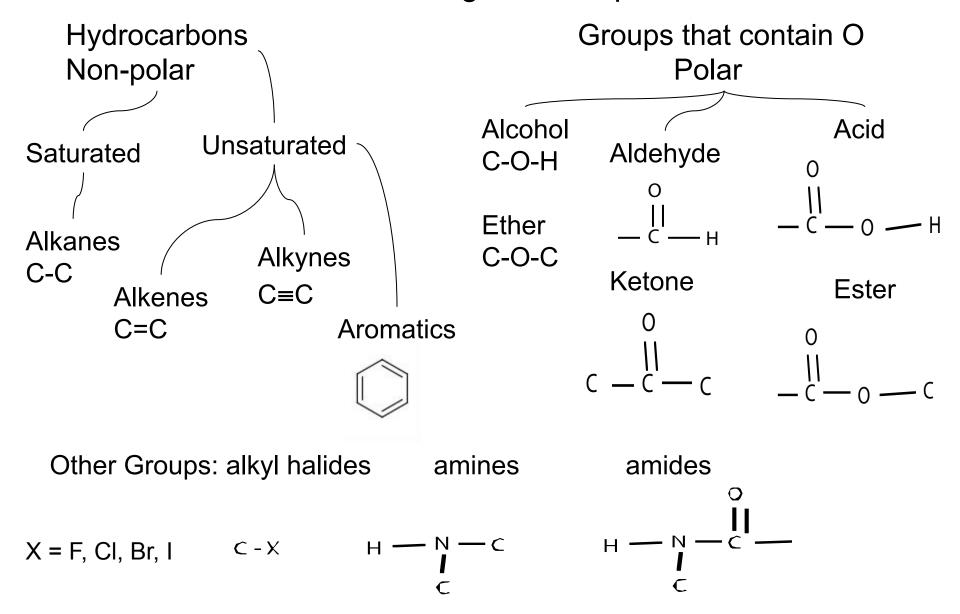
99% of all living organisms and more than 99% of all chemical compounds contain:

carbon hydrogen oxygen

nitrogen phosphorous sulfur

Organic Compounds are Classified by Functional Groups

Functional Groups Are Small Groups of Atoms Within An Organic Compound



General Bonding Rules:

Atom	# of bonding pairs	# of lone pairs
Carbon	4	0
Nitrogen	3	1
Oxygen	2	2
Hydrogen	1	0
F, CI, Br, I	1	3

What rule is followed for each atom, except H?

Organic Compounds can be Big

If you get tired drawing the H's ==> Use **Skeletal Structure**



H's bonded to C are implicit, C's are not labeled.

Acetone is a common organic solvent, e.g., used in finger nail polish remover

Formula = $(CH_3)_2CO$

Draw the Lewis structure.

What is the shape at each C?

Is acetone polar or non-polar?

Is acetone soluble in water?



http://cdn.thebrickblogger.com/wp-content/uploads/2011/01/Acetone.jpg

Aspirin and NSAIDS are Organic Compounds

Identify the functional group(s) in each compound. Why is aspirin more soluble in ethanol than in water?

Hot and Spicy Tastes are Organic Compounds:

Capsaicin, Piperine, Zingerone

Identify the functional group(s) in each compound. How can you get rid of the hot and spicy taste on your tongue?

$$+10$$

Capsaicin - chili peppers

Piperine - black pepper

Zingerone - ginger

Would you eat a food with ARTIFICIAL food coloring or NATURAL food coloring?

In UK, Yellow M&Ms use turmeric rather than Yellow No. 5 Orange M&Ms use β-carotene rather than Yellow No. 6 Red M&Ms use carmine rather than Red No. 40

In US, Blue M&Ms use *phycocyanobilin* (extract from blue-green algae) rather than Blue No. 1. What <u>color</u> is <u>absorbed</u> by this compound?



Phycocyanobilin

Yellow Curcumin (turmeric extract)

http://

turmericextract.com/

http://www.worldofmolecules.com/colors/bcarotene.htm

Red Carmine

(from scale insects)

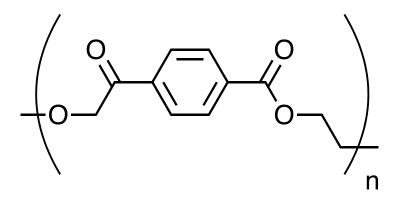
https://en.wikipedia.org/wiki/ Carmine

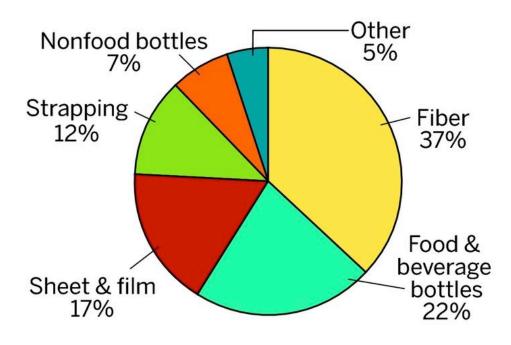
Plastics are Organic Compounds

PET = PolyEthyleneTerephthalate = synthetic fibers (carpet), beverage and food containers

Recyling: soda bottles --> carpet







PET bottles recycled in the U.S. in 2009 = 937 million lb

http://cen.acs.org/articles/89/i38/New-Life-Soda-Bottles.html

Coke Wants a Completely Plant-derived Soda Bottle

(1/23/12, CEN, p. 19, http://cen.acs.org/articles/90/i4/Coke-Plays-Spin-Bottle.html)

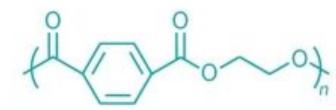


2009: <u>PlantBottle</u> used for Coca-Cola and Dasani water. PlantBottle uses (PET):

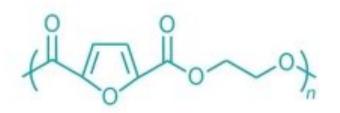
FG + PTA --> PFT

EG = ethylene glycol, PTA= terephthalic acid EG sources = petroleum or ethanol from plants (sugar).

EG from plants = about 30% renewable 2011: Approx. 7 billion PlantBottles made = 6% of its total plastic bottle volume



Polyethylene terephthalate (PET)



Polyethylene furanoate (PEF)

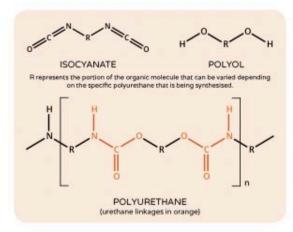
PEF comes from glucose and fructose and is a better O₂ and CO₂ barrier than PET.

THE CHEMISTRY OF THE WORLD CUP BALL



POLYURETHANE COVERING

The surface covering of a football is composed of synthetic leather; in professional footballs, this is made from polyurethane polymers. The World Cup ball is made from six polyurethane panels, which are thermally bonded together. This covering protects the ball and minimises water absorption. In cheaper footballs, the coating can be made from PVC.



Polyurethane is a polymer - a very large molecule built up from many smaller units bonded together. The basic synthesis of polyurethanes involves the addition reaction of isocyanate and polyol molecules to form urethane groups.



NYLON LINING



Several layers of lining are used between the covering of the football and the bladder to improve the bounce and strength of the ball. This lining is made of nylon, another class of polymers also known as polyamides. Polyesters can also be used for this purpose.

BUTYL BLADDER



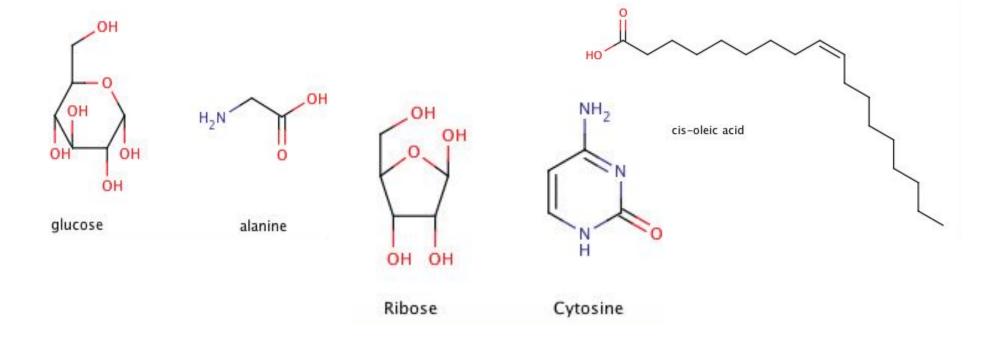
The bladder is the part of the ball in which the air is contained. Butyl rubber is often used because it retains the air better than the other option, latex. However, latex bladders can provide better surface tension.





Biology and Biochemistry is the **Organic Chemistry of Biomolecules**

Biomolecule	Carbohydrates	Proteins	Lipids	Nucleic Acids
Functional Groups	Alcohol Ether Aldehyde Ketone	Amines Acids Other	Alkene Acid Ester	N Base Sugar (ribose) Phosphate



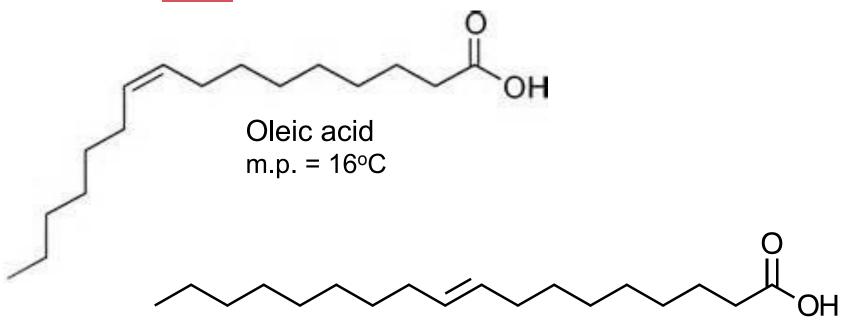
Is It Better to Eat Bent Molecules or Straight Molecules?

Saturated Fats are **Straight**

Unsaturated Fats Are **Bent** or **Straight**!

Trans Fats = **Straight** Unsaturated Fats

Cis Fats = **Bent** Unsaturated Fats



Elaidic acid m.p. = 45°C

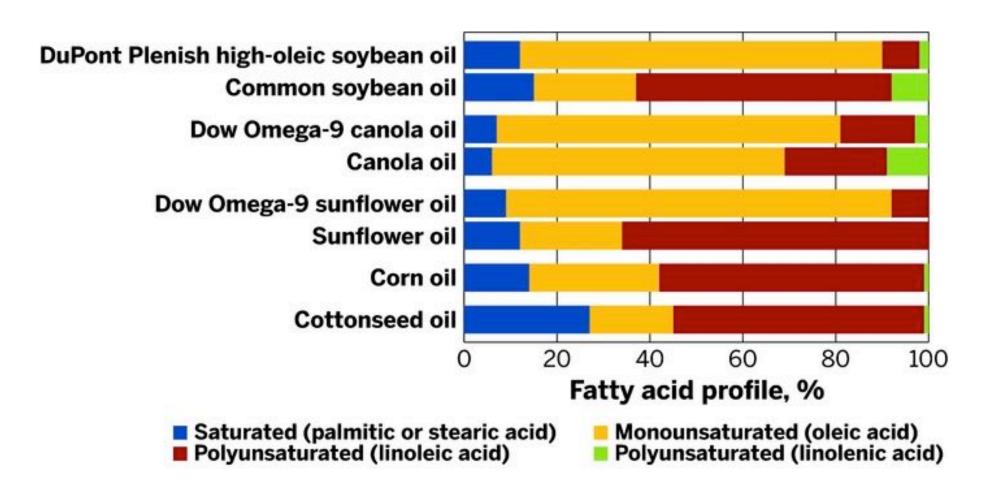
Which fatty acid is better to eat?
Are these two compounds isomers?

http://cen.acs.org/articles/90/i11/Replacing-Trans-Fat.html

3/12/12, CEN, p. 30 Replacing Trans Fat

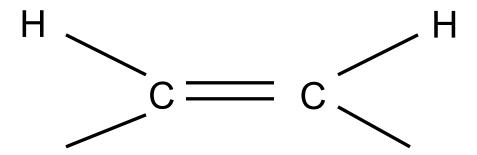
New crops from Dow Chemical and DuPont target food makers looking for stable, heart-healthy oils

New seeds yield crops with higher proportion of monounsaturated oleic acid.



Cis and Trans Isomers

Cis = H's are on same side of C=C double bond



Trans = H's are on opposite side of C=C double bond

$$c = c$$

Fats are used to make Soaps and Detergents

How does soap remove dirt?

What is the difference between solid soap and liquid soap?

<u>Histamines</u> are found in virtually all animal body cells. Certain substances, such as allergens, cause the release of histamines, which cause an inflammatory response (itching, sneezing, runny nose, watery eyes).

<u>Chlor-Trimeton</u> is a 1st generation OTC antihistamine (side effects: drowsiness, psychomotor impairment, dry mouth eyes).

<u>Claritin</u> is a 2nd generation OTC antihistamine (not as likely to cause side effects).

Chlor-trimeton (Chlorphenamine)

What do these three compounds have in common? How do you think an antihistamine works?

Histamine

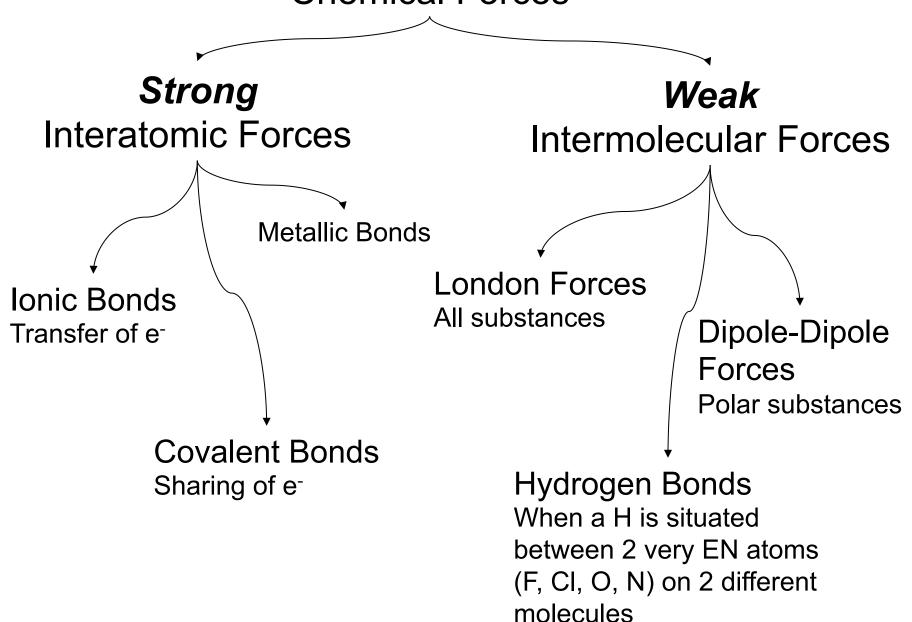
CI

Claritin (Loratadine)

- 1. a. What is the difference between a saturated fat and unsaturated fat?
- b. What is the difference between a trans fat and cis fat?
- 2. a. Circle the functional group(s) in wintergreen (methyl salicylate). Write the name of the functional group next to your circle.

b. You just ate a Wintergreen Lifesaver and don't like the wintergreen taste on your tongue. How do you get rid of the taste?

Chemical Forces



Intermolecular (IM) Forces Hold Atoms/Molecules Together in its State of Matter

At room temperature, H_2O is a liquid and H_2S is a gas. Explain using IM forces. (Liquid = Stronger IM forces; Gas = Weaker IM forces)

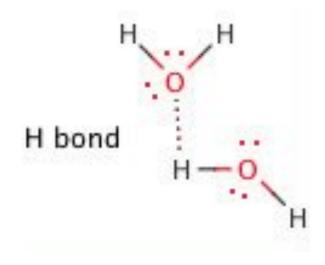
To identify IM forces in a substance:

- 1. Draw Lewis structure.
- 2. Determine shape (VSEPR theory).
- 3. Determine polarity of molecule.
- 4. Determine IM forces.

London forces

Dipole-dipole forces (because H₂O is polar)

H bonds



Polarity Determines Intermolecular Forces IM Forces Determines Solubility

Identify the intermolecular forces in CO_2 Is CO_2 soluble in water? Identify the intermolecular forces between CO_2 and water.

Structure: O=C=O How many lone pairs are missing?

Shape = linear

Polarity = Non-polar

IM forces = London forces only

Polarity Determines Intermolecular Forces IM Forces Determines Solubility

Identify the intermolecular forces in Acetone What organic functional group(s) is/are in acetone? Is acetone soluble in water? Identify the intermolecular forces between acetone and water.

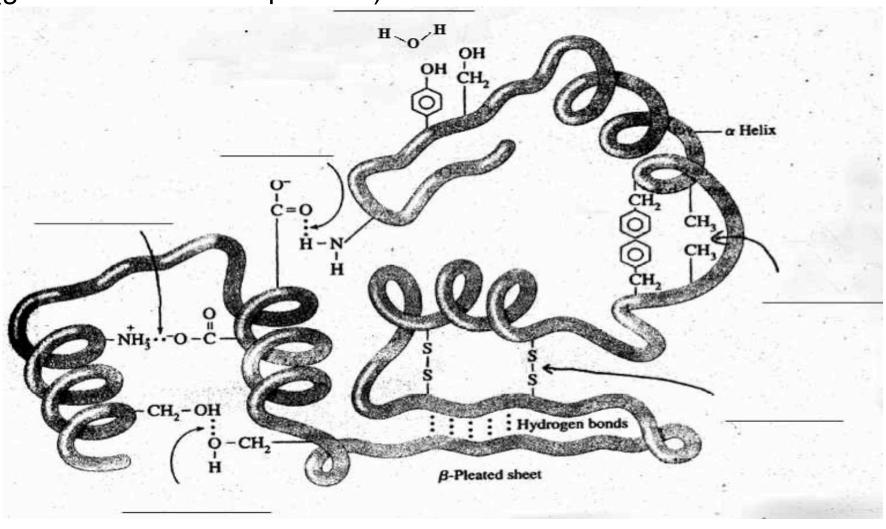
- 1. What is the difference between a saturated fat and unsaturated fat?
- 2. Naproxen is a common over-the-counter (OTC) non-steroidal anti-inflammatory drug (NSAID). Circle the functional group(s) in Naproxen. Write the name of the functional group next to your circle.

Is Naproxen soluble in water? Give reasons.

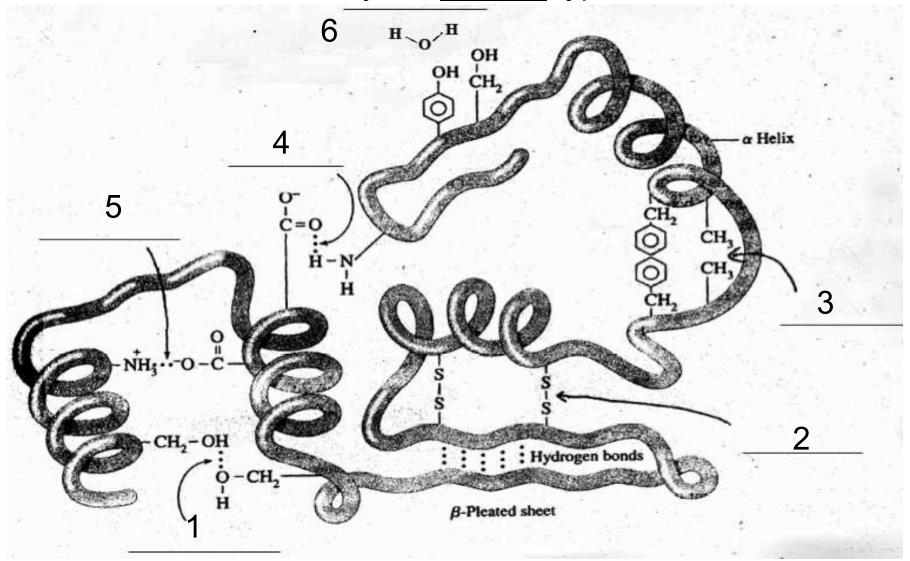
Hydrogen Bonds are Important in Biology

DNA base pairing (A-T, C-G) and double helix shape are due to H bonds.

 2° protein structure (α helix and β sheet) and 3° protein structure (globular and fibrous proteins) are due to H bonds.



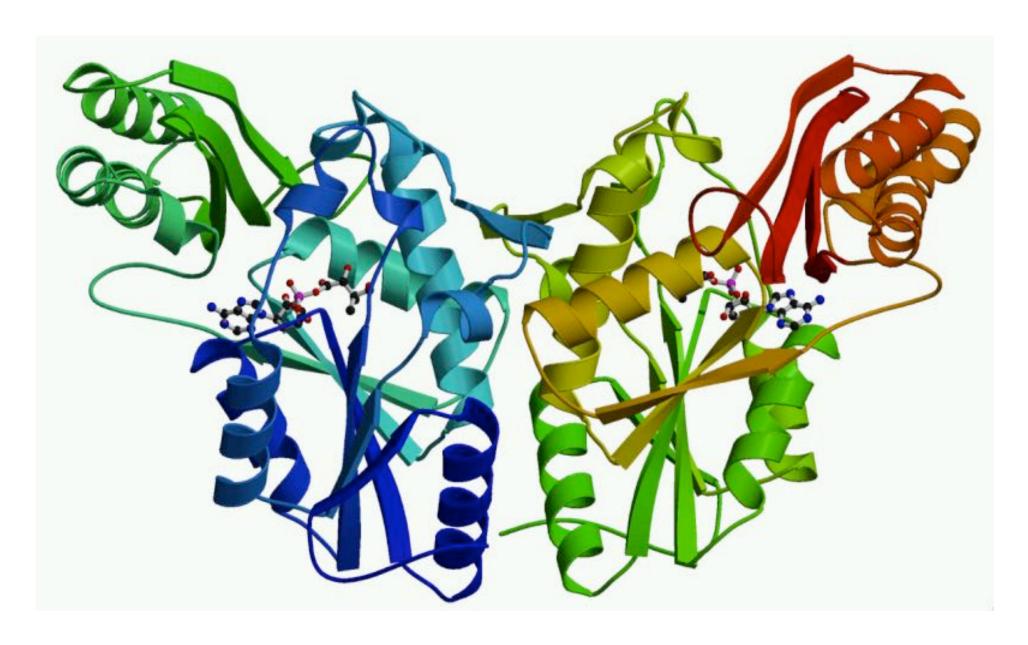
Note the arrows that point to specific interactions in the protein. Next to each arrow, identify the <u>specific</u> type of chemical force.



As the protein is heated, which specific interaction in the protein do you think will break first? Give reasons.

PanC enzyme (involved in Vitamin B5 biosynthesis)

http://biomedicalcomputationreview.org/content/crescendo-protein-structures



Polarity Determines Intermolecular Forces IM Forces Determines Solubility

Dyes and fabrics: FDC Red No. 40 and cotton. Identify the intermolecular forces between the dye and fabric. (See Lab 9 Problem 4)

Two Properties of Dyes:

- 1. <u>Fastness</u> the ability of a dye to stick to a fabric after repeated washings
- 2. Levelness the uniformity of a dye on a fabric



Try This! Find white fabrics.

Dye with food colors.

ID chemical forces that bind dye to fabric.

http://www.howtotiedye.org/tie-dye-t-shirt/

"Blue jeans might just be the world's most popular piece of clothing." C&EN, 10/24/11, p. 44.

Indigo is the dye used in blue jeans.

Indigo is <u>insoluble</u> in water. To dye cotton, indigo is <u>reduced</u> to **leucoindigo** (water soluble, yellow dye, pH 11.5-12 for yarn absorption). Once the cotton is dyed with leucoindigo, it is exposed to O_2 in air which <u>oxidizes</u> the <u>yellow</u> leucoindigo to blue indigo.

Cotton is the Most Used Textile Fiber in the World

(56% of all fibers for apparel and home furnishings) Cotton is celluose (a complex carbohydrate).

http://www.engr.utk.edu/mse/Textiles/Cotton%20fibers.htm

leucoindigo (yellow) at pH 12

What chemical force(s) bind indigo to cotton?

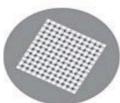
Clothes: Textile production involves Chemistry

> 8,000 chemicals to make the 400 billion m² of fabric sold per year pair of jeans requires about 1,800 gal of water; a T-shirt takes 700 gal.



Step 1: YARN

Oils to reduce friction during spinning



Step 2: FABRIC PRODUCTION

Sizing chemicals, lubricants, solvents such as benzene, adhesives, and binders



Step 3: PRE-TREATMENT

Surfactants such as alkylphenol ethoxylates, solvents, bases for cleaning fabric, bleaches to prepare for dyeing



Step 4: DYEING AND PRINTING

Heavy metal fixing agents and dyestuffs, polymers and plasticizers for printing, detergents



Step 5: FINISHING

Softening using ammonium compounds, silicones, polyurethanes; crease resistance using a formaldehyde-based resin; water and stain resistance using fluorocarbons

http://cen.acs.org/articles/93/i41/Cutting-Textile-Pollution.html

Picric Acid is Used as a Wool Dye (Brown)

Picric acid largest use is as an explosive

What chemical force binds picric acid to wool?

One Dye Does Not Work for Every Fabric

Dye Type	Description	Fabric type	Conditions or Example
Acid	Water-soluble anionic dyes	Wool nylon	Neutral or acid
Basic	Water-soluble cationic dyes	Acrylic Some polyesters	Acetic acid helps uptake of dye
Direct	Water-soluble anionic cpds	Cotton Rayon	Neutral or sl basic
Disperse	Not water-soluble	Polyester acetate	Dye T=130°C and high P
Reactive	Water-soluble anionic cpds	Cotton	Covalent bond to fiber (permanent)
Sulfur	Organic cpds containing S or Na ₂ S	Cotton	Developed dye for dark colors
Vat	Not water-soluble	Cotton	Basic solution Indigo

http://cen.acs.org/articles/89/i39/Making-Changes-Printing.html

9/26/11, CEN, p. 18 Ink Jet Printing Dyes and Colorants

1980's: **black** azo dyes: cheap, easy to make but bleeds into low quality paper and faded with time.

1990's: color ink pigments: high color strength and image permanence but hard to make stable dispersions of insoluble material that could be sprayed through tiny jets and agglomerate on paper

Key: attach pigment to diazonium salt to improve solubility

X = halide; R = carboxylate, ammonium species, fatty acid chain, sulfonyl, or other groups

http://cen.acs.org/articles/89/i31/Rethinking-Deinking.html

8/1/11, CEN, p. 42 "Rethinking Deinking"

Paper is de-inked during recycling.

Analog ink is oil based; digital ink is water based.

When you have a mixture of paper, how is each ink removed?

Printing Methods: Conventional (analog) and Digital.

Major markets: newspapers, magazines, most books

Offset lithography: Image is transferred to a printing plate using solvent-based inks. The image is then transferred to a rubber blanket and finally to paper.

<u>Gravure</u>: Image is engraved into a metal cylinder. The recesses are filled with a water- or solvent-based ink, which is then pressed onto paper.

<u>Flexography</u>: Raised image is created on flexible polymer plate. Resulting relief plate is rolled through water-based ink and then transferred first to a series of metal cylinders and finally to paper

Major markets: short-run book printing, direct mail, packaging, photo products Ink-jet: Image is created by jetting droplets of water-based or waterless ink onto paper. Liquid electrophotography: Image is produced by scanning a laser beam across a photoconductor-coated drum to selectively remove charge. Liquid toner particles are transferred to discharged areas on the drum, then to a rubber blanket, and finally to paper. Laser: Image is produced by scanning a laser beam across a drum coated with organic

photoconductor to selectively remove charge. Charged areas attract dry toner particles, which are then fused onto paper.

Wrinkle-Free Cotton (C&EN, 12/2/13, p. 32)

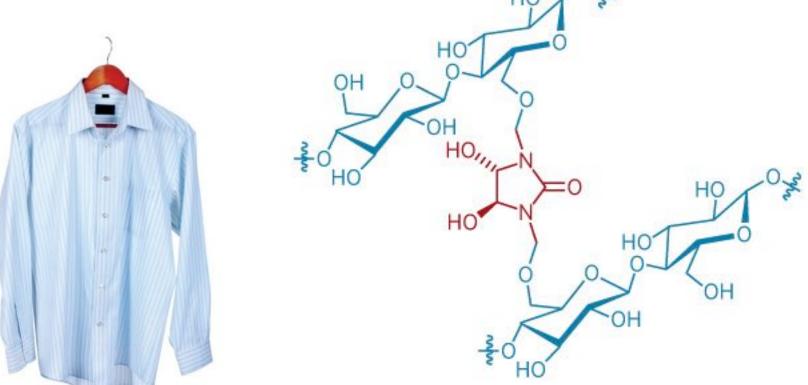
http://cen.acs.org/articles/91/i48/Wrinkle-Free-Cotton.html

Cotton is made of numerous parallel chains of cellulose.

These chains are held together by weak hydrogen bonds.

H bonds break in warm dryer and re-form as chains shift into new

positions.

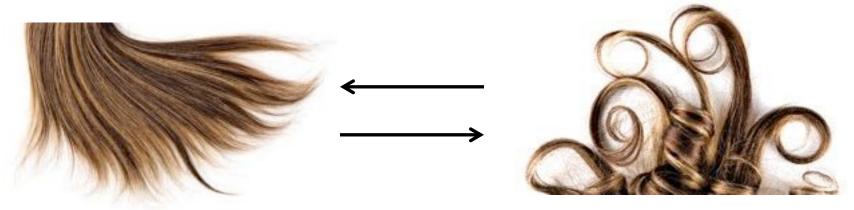


Treat fabric with molecules that *cross-link* the chains to permanently hold them in place. (DMDHEU = dimethylol dihydroxyethylene urea)

Hair Staighteners

http://cen.acs.org/articles/88/i45/Hair-Straighteners.html

Break bonds to change shape



Hair is a fiber made of keratin (a protein).

Hair gets its structure from two types of bonds in Keratin:

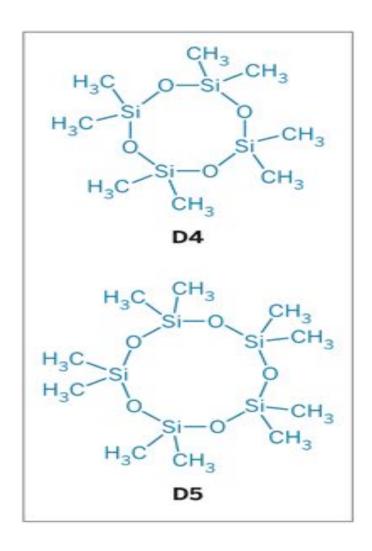
- 1. Disulfide bonds (covalent)
- 2. Hydrogen bonds (intermolecular)

Cross-link amino acids in hair fibers to keep shape. Straighteners: formaldehyde (Brazilian Blowout)

Ammonium thioglycolate (Japan)

Personal Care Products

Si compounds give skin creams a silky nongreasy feel and hair a luxurious bounce and shine.





50% of U.S. market for silicones are used in Antiperspirants and Deodorants

D4 = octamethylcyclotetrasiloxane. Potentially toxic and can wash off hair and skin and bioaccumulative (build up in environment).

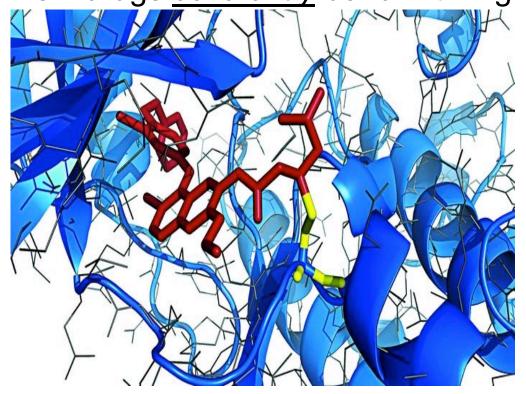
Replaced by:

D5 = decamethylcyclopentasiloxane

http://cen.acs.org/articles/89/i18/Storm-Over-Silicones.html

http://cen.acs.org/articles/89/i36/Covalent-Drugs-Form-Long-Lived.html

9/5/11, CEN, p. 19 "Covalent Drugs Form Long-Lived Ties" Small molecule drugs bind to protein target via *IM forces*. New drugs *covalently* bond with high selectivity and low toxicity.



Neratinib (red), a Pfizer drug candidate, forms a covalent bond with a cysteine (yellow) of epidermal growth factor receptor (blue).