Chem 1B Objective 1:
Identify organic functional groups, draw skeletal structures, and distinguish between the same compound, isomers, resonance structures, and different compounds.

Key ideas:
Functional groups – a small group of 2 to 5 atoms within an organic compound that has specific properties.
See General bonding rules for Organic compounds.

Isomers – same chemical formula, different bonding

Covalent bond - electrons shared between 2 atoms only --> localized electrons.

Electrons shared between 3 or more atoms – delocalized electrons. Need to show resonance structures to represent delocalized electrons. Experimental evidence – see IR.

Most Compounds are Organic (16 million known)
Organic compounds contain: carbon, hydrogen, oxygen, nitrogen, phosphorous, and sulfur

General Bonding Rules:

Atom	# of bonding pairs	# of lone pairs
C	4	0
N	3	1
O	2	2
H	1	0
F, Cl, Br, I	1	3

Biological Molecules are Organic Compounds

Carbohydrates
Lipids
Proteins
Nucleic acids

Functional Groups Are Small Groups of Atoms Within An Organic Compound

Hydrocarbons
Non-polar

Saturated

Alkanes
C-C

Unsaturated

Alkenes
C=C

Alkynes
C≡C

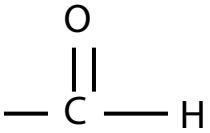
Aromatics

Groups that contain O
Polar

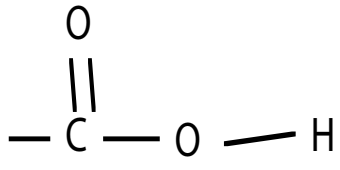
Alcohol
C-O-H

Ether
C-O-C

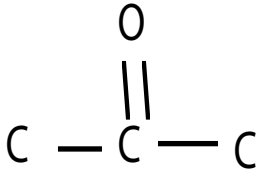
Aldehyde



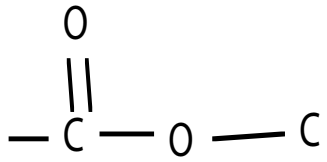
Acid



Ketone

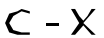


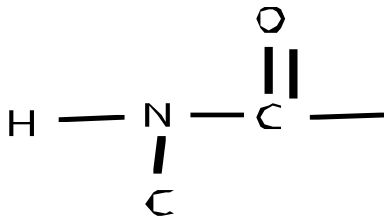
Ester



Other Groups: alkyl halides amines amides

X = F, Cl, Br, I





How Do You Determine How Atoms Are Bonded Together In A Compound?

(In other words, how do you determine the structure of a compound?)

X-ray diffraction

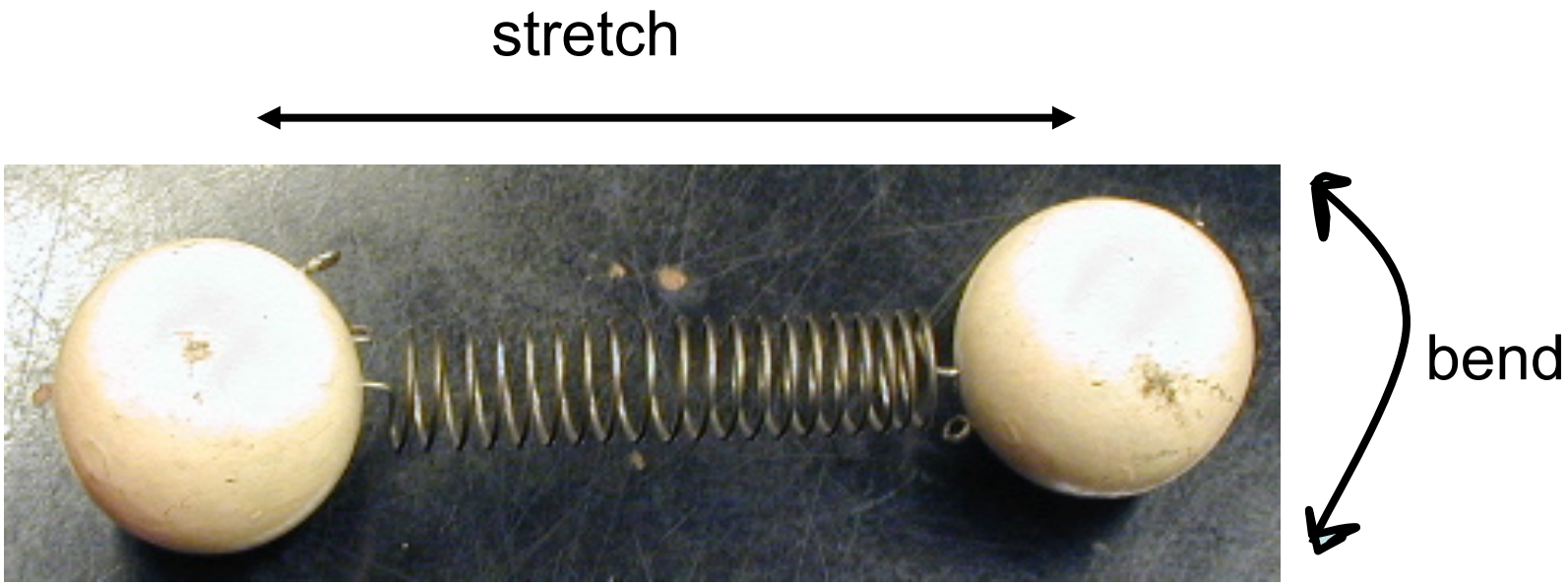
Infrared (IR) spectroscopy – *we will use in Lab 1*

Nuclear magnetic resonance (NMR) spectroscopy

UV-Vis spectroscopy

Mass spectrometry

Bond Types are determined by IR Spectroscopy



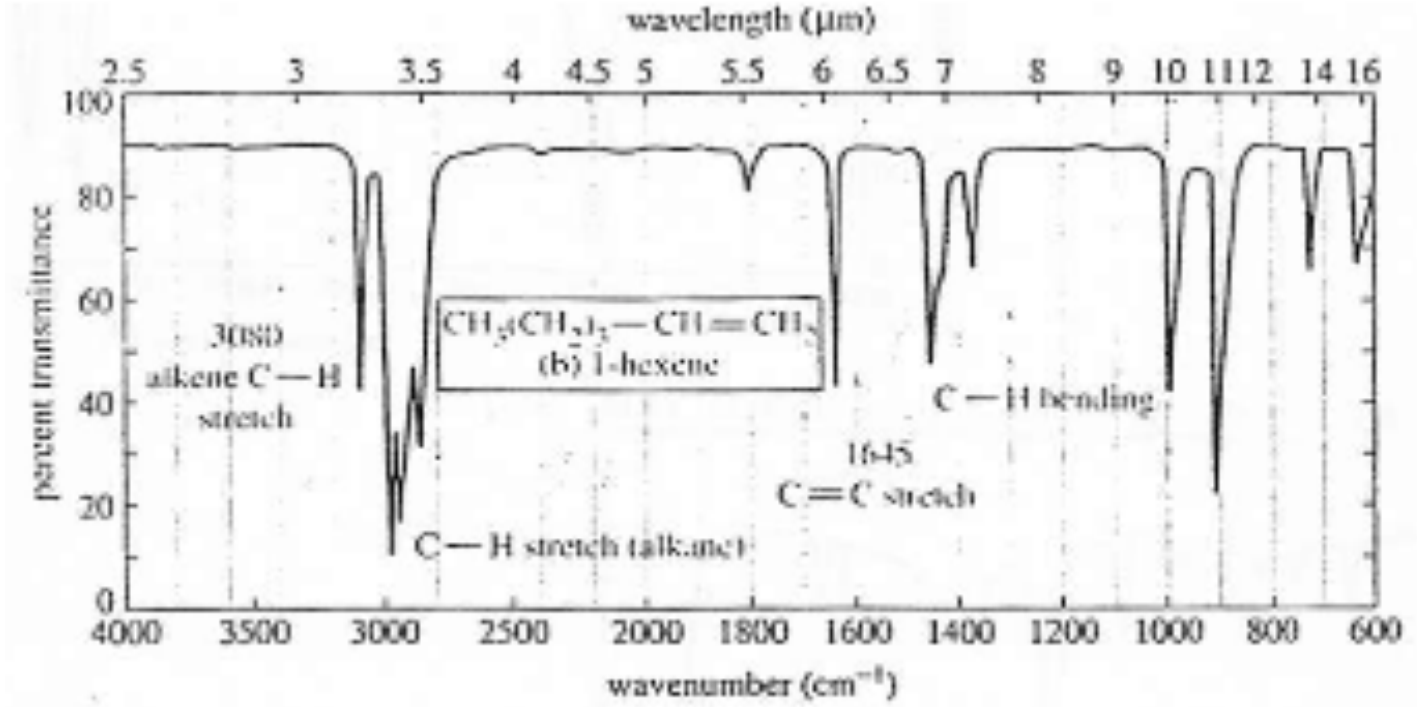
http://teacher.pas.rochester.edu/PhysicsDemos/Mechanics/MA_ElasticSolids/MA-01/MA-01.html

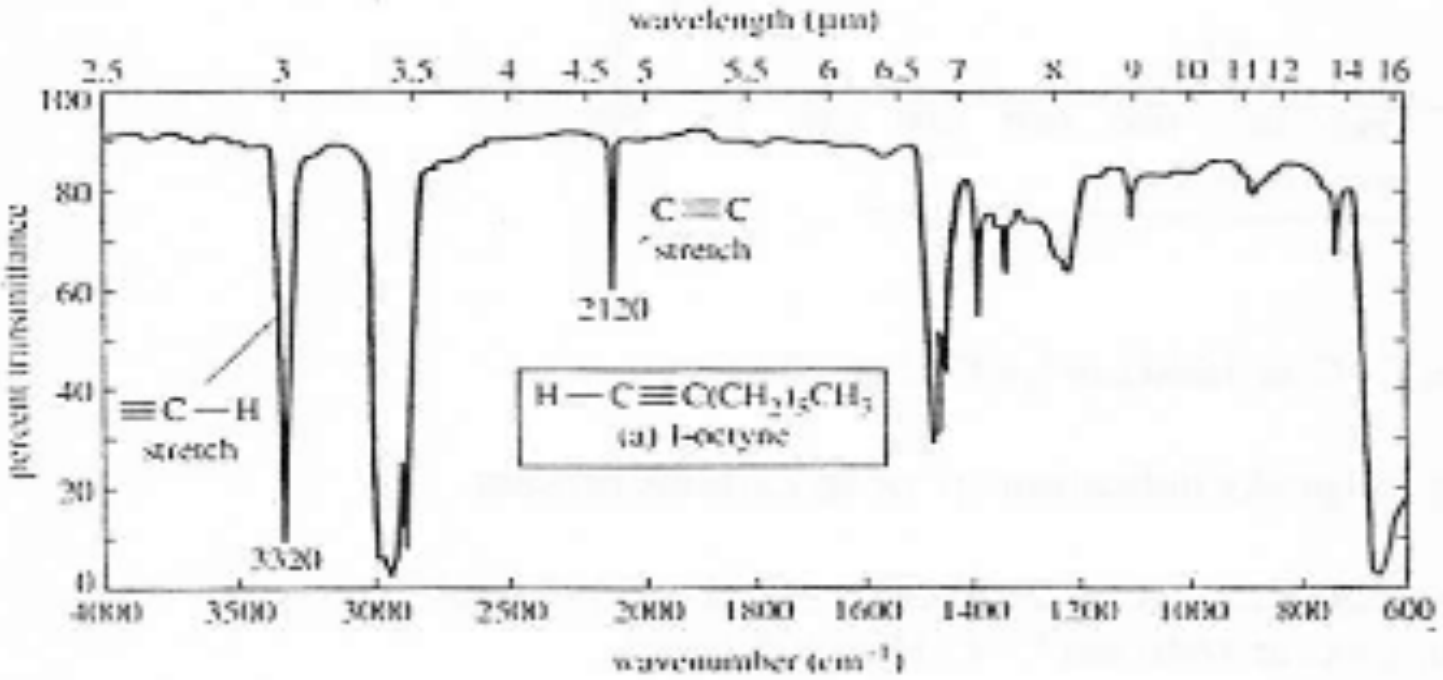
Which bond type requires the most energy to stretch?
Hint: Hooke's law (physics) – spring strength, mass of ball

1. a. C-C b. C=C c. C≡C

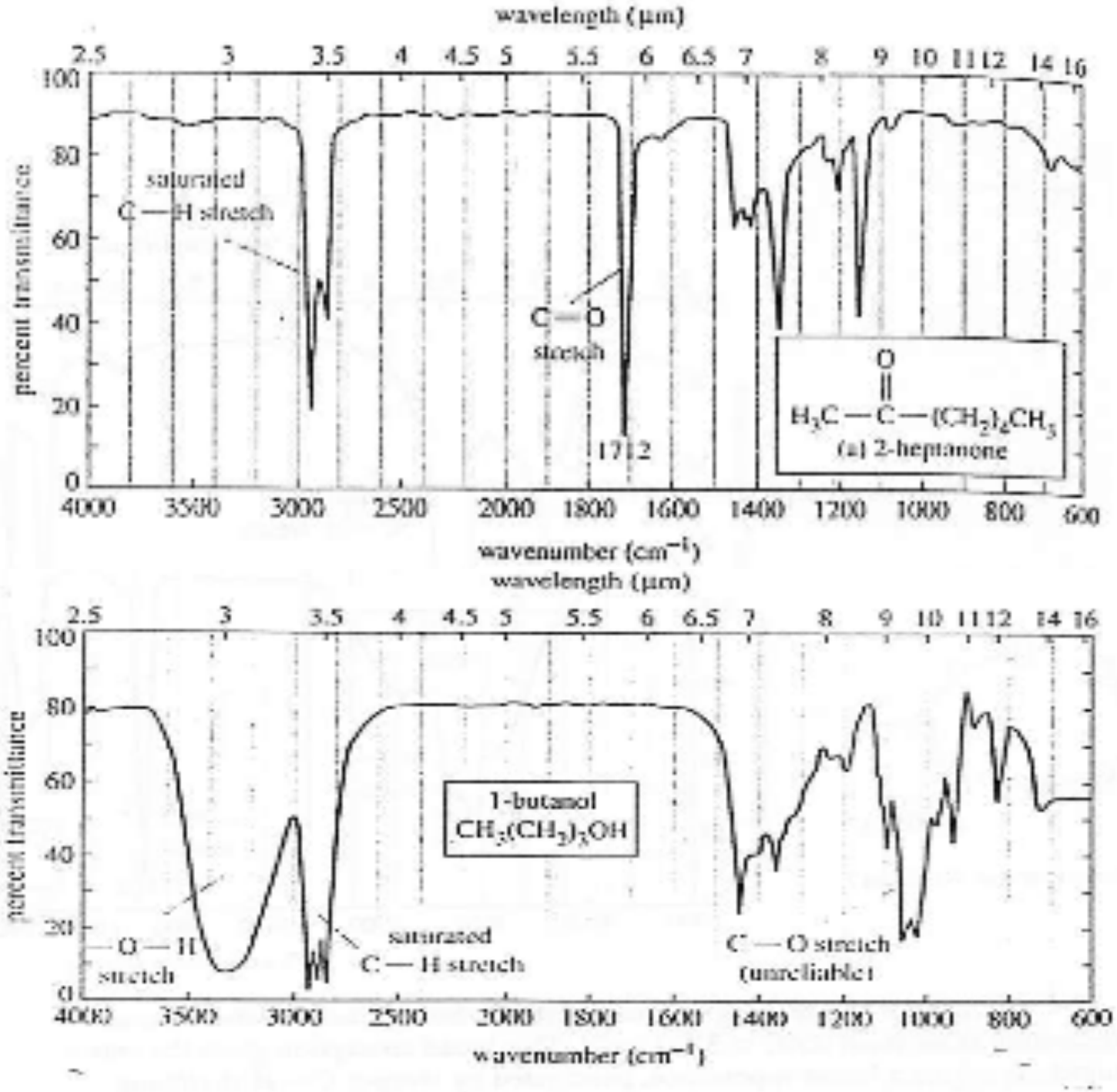
2. a. C-H b. O-H

IR Spectra


wavelength (μm)
2.5 3 3.5 4 4.5 5 5.5 6 6.5 7 8 9 10 11 12 14 16
100 80 60 40 20 0
percent transmittance
3080
alkene C—H
stretch
CH3(CH2)3—CH=CH2
(b) 1-hexene
C—H stretch (alkane)
1645
C=C stretch
C—H bending
4000 3500 3000 2500 2000 1800 1600 1400 1200 1000 800 600
wavenumber (cm−1)


wavelength (μm)
2.5 3 3.5 4 4.5 5 5.5 6 6.5 7 8 9 10 11 12 14 16
100 80 60 40 20 0
percent transmittance
C≡C
stretch
2120
≡C—H
stretch
3320
H—C≡C(CH2)3CH3
(a) 1-octyne
4000 3500 3000 2500 2000 1800 1600 1400 1200 1000 800 600
wavenumber (cm−1)

IR Spectra


wavelength (μm)
2.5 3 3.5 4 4.5 5 5.5 6 6.5 7 8 9 10 11 12 14 16
100 80 60 40 20 0
percent transmittance
saturated C—H stretch
C—O stretch
1712
O
H3C—C—(CH2)4CH3
(a) 2-heptanone
4000 3500 3000 2500 2000 1800 1600 1400 1200 1000 800 600
wavenumber (cm−1)
wavelength (μm)
2.5 3 3.5 4 4.5 5 5.5 6 6.5 7 8 9 10 11 12 14 16
100 80 60 40 20 0
percent transmittance
1-butanol
CH3(CH2)3OH
O—H stretch
saturated C—H stretch
C—O stretch (unreliable)
4000 3500 3000 2500 2000 1800 1600 1400 1200 1000 800 600
wavenumber (cm−1)

Name and Suffix tells you # of C and Functional Group

Number of Carbons: see Chang, 6th ed., Chapter 11, Table 11.1, p. 366.

1 carbon = CH_4 = methane
2 carbons = C_2H_6 = ethane
3 carbons = C_3H_8 = propane
4 carbons = C_4H_{10} = butane
5 carbons = C_5H_{12} = pentane
6 carbons = C_6H_{14} = hexane

Suffix	Functional Group	One Carbon Cpd	Two Carbon Cpd
-ane	alkane	methane	ethane
-yl	alkyl group (alkane - 1 H)	methyl	ethyl
-ene	alkene		ethene (ethylene)
-yne	alkyne		ethyne (acetylene)
-ol	alcohol	methyl alcohol methanol	ethyl alcohol ethanol
-al	aldehyde		ethanal (acetaldehde)
-one	ketone		3 C: propanone (acetone)
-oic acid	acid	Methanoic acid (formic acid)	Ethanoic acid (acetic acid)

Name and Suffix tells you about functional group.

Ethane - 1 H ---> Ethyl

C_2H_6 - 1 H ---> C_2H_5

Check bonding of C_2H_5.

One C needs one more bond → bond to functional group

C_2H_5OH = ethyl alcohol = ethanol

Cholesterol = -ol tells you this compound has an alcohol group.

Acetone = -one tells you this compound has a ketone group.

Octane = -ane tells you this compound is an alkane.

Determine the number of carbon atoms and functional group based on the name. Draw the Lewis structure. (There may be **ISOMERS** - more than one way to draw a structure of a compound.)

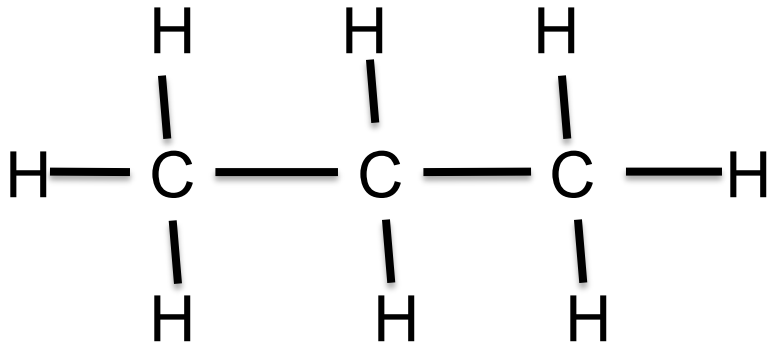
1. Propanol is a 3 carbon alcohol
Propane = 3 carbon alkane, -ol for alcohol functional group.

2. Hexanone

3. Butadiene

4. Pentanal

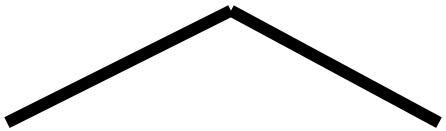
Big Organic Compounds have a ***LOT*** of H's



(you get tired of drawing all the H's in the structure)

Skeletal structure = shortcut to Lewis structure

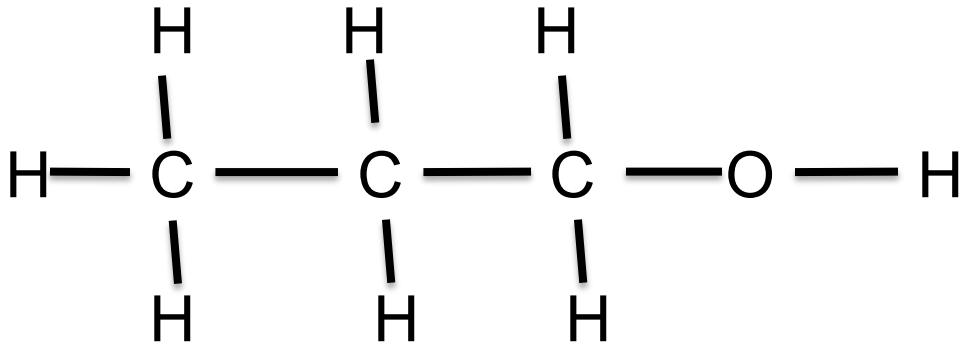
Each line is a bond



A C is at the end of each bond

The H's bonded to C are <u>not</u> drawn

Big Organic Compounds have a ***LOT*** of H's



(you get tired of drawing all the H's in the structure)

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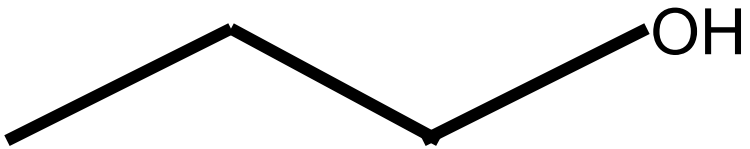
Each line is a bond



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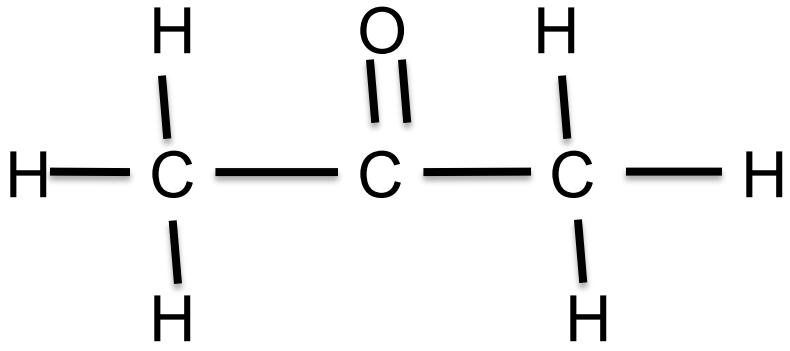


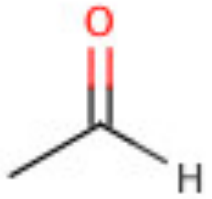
Draw Skeletal structure of this compound.

What happens to alcohol after you drink it?

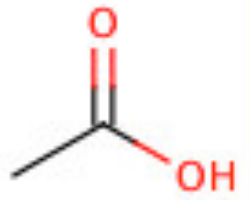
Draw Lewis structure of each compound.

Identify the functional group in each compound:

a. Alkene b. alcohol c. acid d. aldehyde



a. Alkene b. alcohol c. acid d. aldehyde



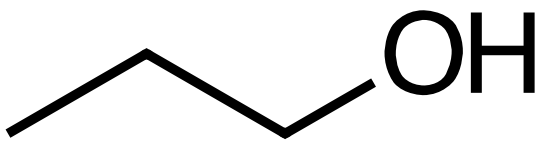
a. Alkene b. alcohol c. acid d. aldehyde

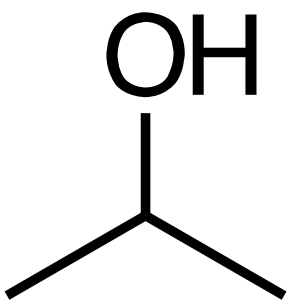
Hint: draw in the H's

Objective: Identify isomers vs. different cpd

Isomers Have the **Same** Chemical Formula but Different **Connectivity** (***Structural Isomers***)

Propanol has two isomers.





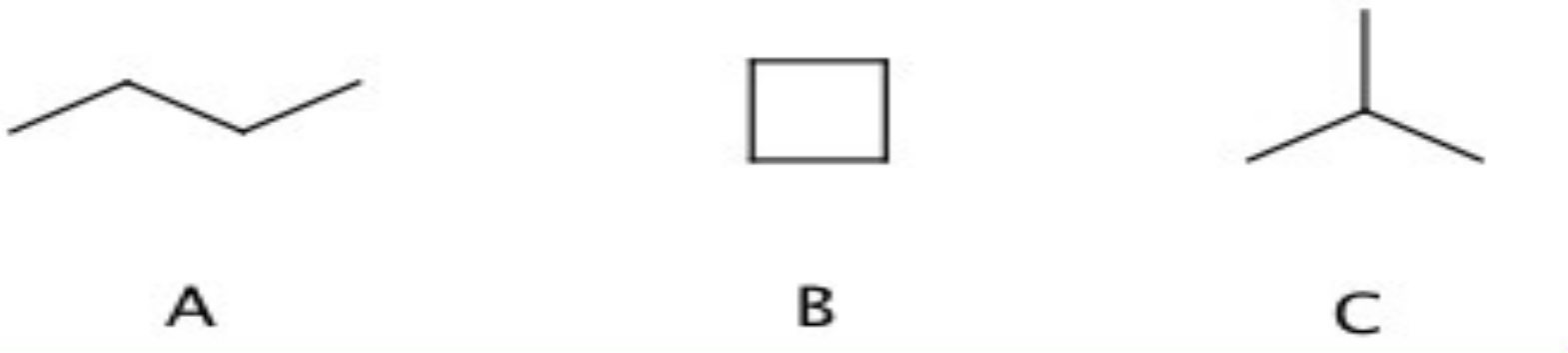
Do these 2 structures have the same chemical formula?
Is the bonding the same? Check bond type (e.g., C-H bond, C-C bond, C-O bond) on each C.

Objective: Identify isomers vs. different cpd

Isomers Have the **Same** Chemical Formula but Different **Connectivity** (***Structural Isomers***)

Butane, C_4H_{10}, has two structural isomers. Which are the two isomers?

a. A and B
b. A and C
c. B and C

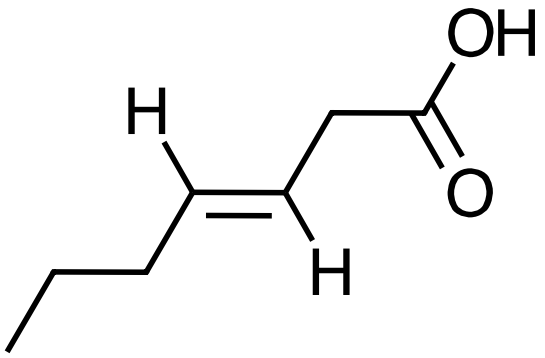


Hint: Same chemical formula? (draw in the H's)
Is the bonding the same?

<u>Objective:</u> Identify isomers vs. different cpd

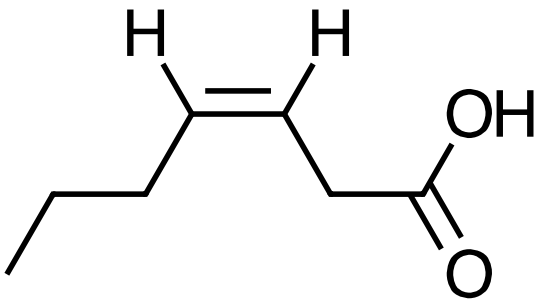
<u>Stereoisomers</u> Have the <u>Same</u> Chemical Formula, <u>Same</u> Connectivity but <u>Different</u> Orientation in Space

Example: cis and trans isomers



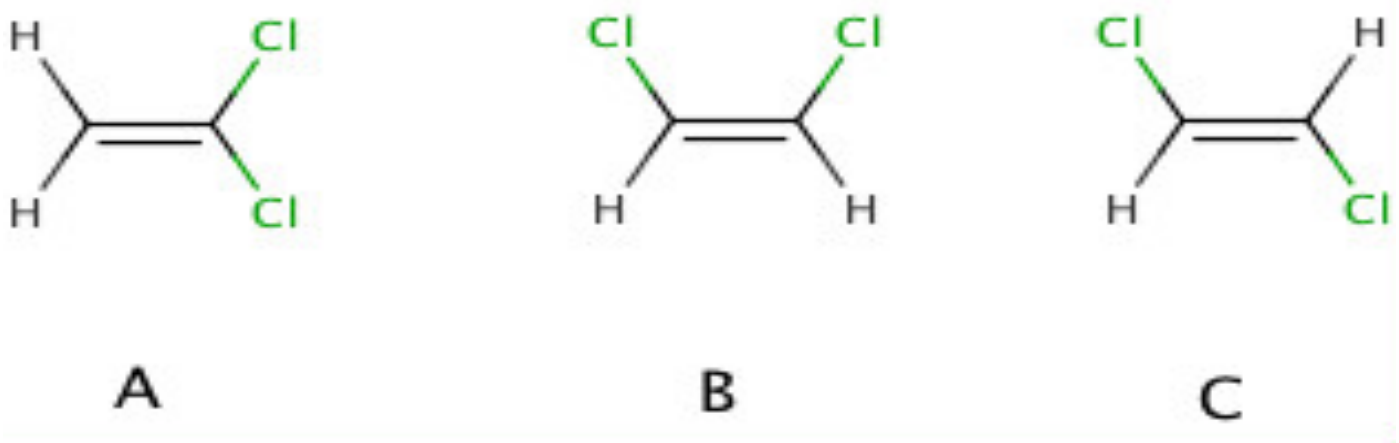
Trans fatty acid – H's across from each other

Compare H's bonded to each C in C=C bond



Cis fatty acid – H's nearest each other.

$C_2H_2Cl_2$ has three isomers.
One isomer is a solvent for waxes and resins.
Another isomer was a precursor for cling wrap (Saran wrap) but is mainly used in semiconductor fabrication.

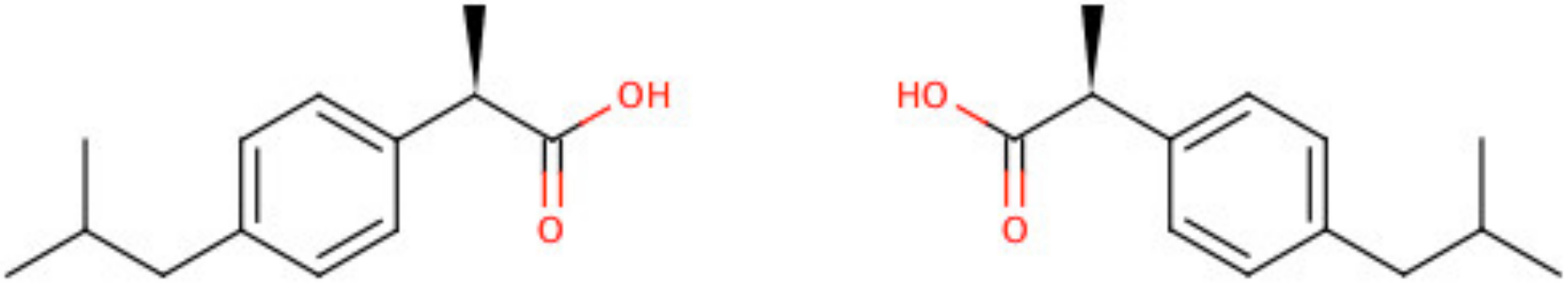


a. Which isomers are structural isomers?
(i) A and B (ii) A and C (iii) B and C

b. Which isomers are stereoisomers?
(i) A and B (ii) A and C (iii) B and C

Enantiomers are mirror image stereoisomers that are not superimposable in each other.

- Left hand and right hand are enantiomers
- Ibuprofen has 2 enantiomers: one relieves pain, the other is inactive (http://en.wikipedia.org/wiki/Ibuprofen)



Determine Properties from Bond Type
Diamonds are Hard; Gold is Soft

What bond type involves localized electrons (the sharing of electrons between 2 atoms)?

a. Ionic bond
b. covalent bond
c. metallic bond
d. H bond

How many electrons are shared between 2 atoms in a single covalent bond?

a. 2
b. 4
c. 6
d. 8

Name one property of a substance due to localized electrons.

Determine Properties from Bond Type

Diamonds are Hard; Gold is Soft

What bond type involves delocalized electrons (the sharing of electrons between 3 or more atoms)?

a. Ionic bond
b. covalent bond
c. metallic bond
d. H bond

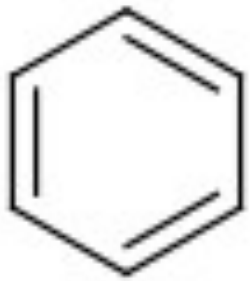
Name one property of a substance due to delocalized electrons.

Determine structure from experimental data

Benzene, C_6H_6, is a common organic solvent.

Experiments show benzene is a 6 carbon ring with 6 carbon-carbon bonds of the same length (140 pm) and 6 C-H bonds.

Draw the Lewis structure of benzene. Does the Lewis structure fit the experimental data? Give reasons.



Lewis structure: 3 C-C bonds and 3 C=C bonds.

C-C longer than C=C .

(Experiment: C-C 154 pm, C=C 134 pm)

Structure does ***NOT*** match the experimental data.

Determine structure from experimental data

Benzene, C_6H_6, is a common organic solvent.

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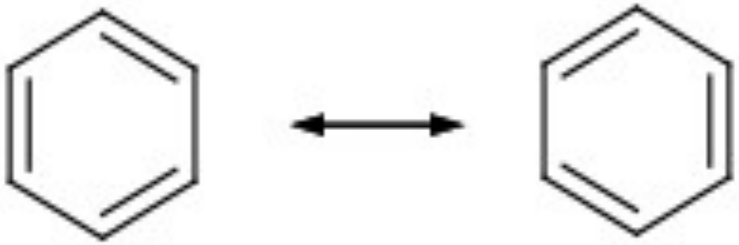


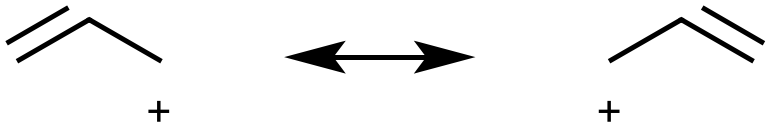
Electrons in the double bonds are shared by the 6 C atoms in ring = delocalized electrons.

Draw 2 **Resonance Structures** to show delocalized electrons.

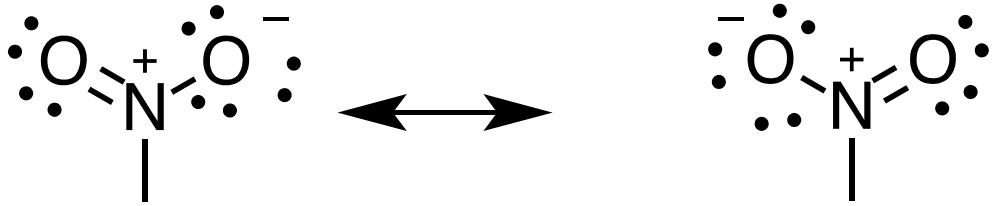
Note: you need experimental evidence of delocalized electrons.

Resonance Structures:

- A Lewis structure shows localized electrons (it does **not** show *delocalized* electrons)
- Each resonance structure has the **same** bonding (no isomers)
- Double bonds or lone pairs or (+) or (-) charge change positions in resonance structures



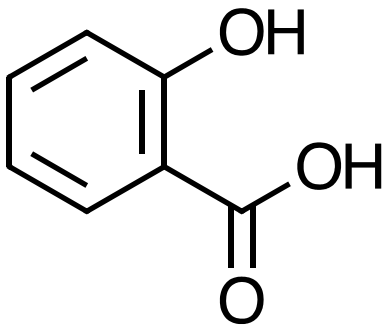
Is each C-C bond the same length?



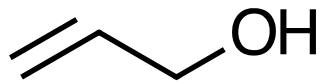
Is each N-O bond the same length?

Over how many atoms are electrons shared?

(from a previous exam) Salicylic acid and 1-propene-3-ol have carbon-carbon double bonds. You measure the IR spectrum of each compound. The C=C peak in salicylic acid is at a lower energy than the C=C peak in 1-propene-3-ol. Give reasons.



salicylic acid



1-propene-3-ol

Determine structure from experimental data

(from Spring 2009 Exam 1) You are trying to determine the identity of an organic ion. So far, your analysis shows that the compound contains:

(i) C and H and O with chemical formula $C_2H_3O_2$,

(ii) Three HCH bond angles and three CCH bond angles of 109.5^o. (Note: methane, CH_4, has four HCH bond angles.)

(iii) Two carbon-oxygen bonds of length 1.26 Angstroms. (Note: A carbon-oxygen single bond has a bond length of 1.34 Angstroms. A carbon-oxygen double bond has a bond length of 1.20 Angstroms.)

Bond Strength Determines Reactivity.

What makes a bond strong or weak? What does d tell you?

Bond	d, pm	ΔH, kcal/ mole	Bond	d, pm	ΔH, kcal/ mole	Bond	d, pm	ΔH, kcal/ mole
C-H	109	99	C-C	154	83	C-O	143	94
O-H	96	104	C=C	134	146	C=O	120	177
N-H	101	101	C≡C	120	201	C≡O	113	256
H-F	92	136	C-F	135	116	C-N	147	73
H-Cl	127	103	C-Cl	177	81	C=N	129	147
H-Br	141	87.5	C-Br	194	68	C≡N	116	212
H-I	161	71	C-I	214	51	N-O	140	48
						N=O	121	145

Note: Average bond energies. Some bonds show considerable variability.

Determine Properties from Bond Type (from Chem 1A)

Do Explosives Have Strong Bonds or Weak Bonds?

http://blogs.sfweekly.com/exhibitionist/2012/04/blowing_up_jj.php

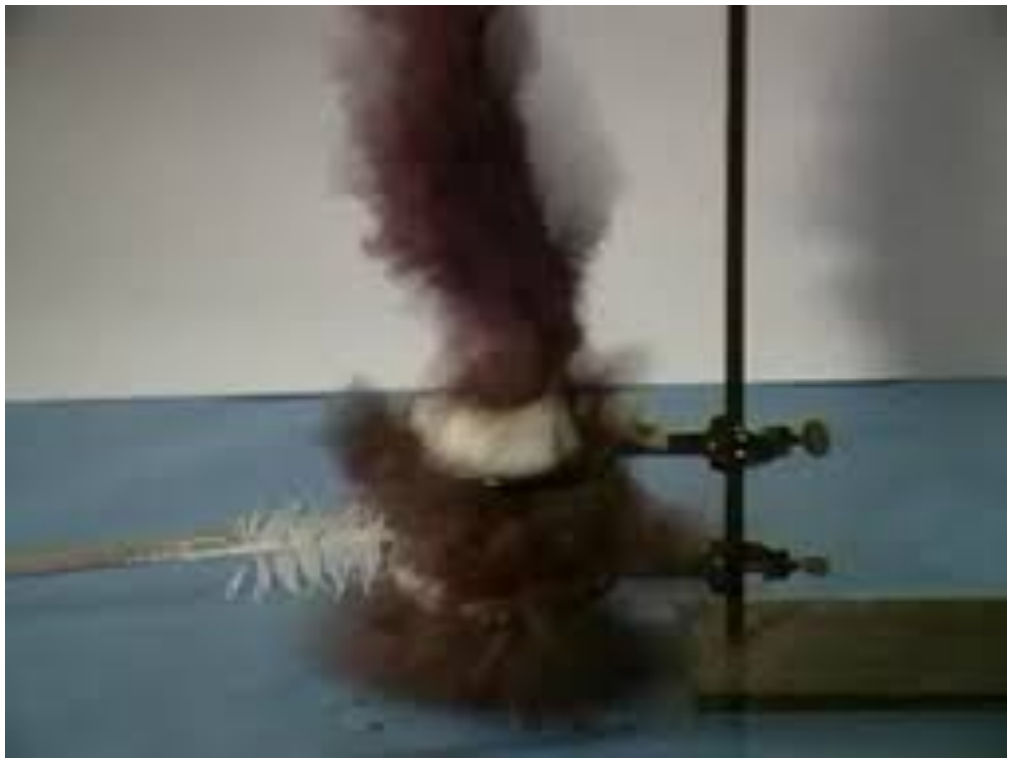
http://www.turbosquid.com/FullPreview/Index.cfm/ID/192192

Determine Properties from Bond Type (from Chem 1A)

Do Explosives Have Strong Bonds or Weak Bonds?

Nitrogen triiodide decomposes ***explosively*** with the touch of a ___.

$$NI_3 \rightarrow N_2 + I_2$$



http://www.openscience.org/blog/?p=95

Which bonds are strong?

Which bonds are weak?

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

$2\ NI_3\ (s) \rightarrow N_2\ (g) + 3\ I_2\ (g)\ (-290\ kJ/mol)$

http://pubs.rsc.org/en/Content/ArticleLanding/1989/C3/C39890001461#!divAbstract

$\Delta H_{formation}$ of $NI_3 \bullet NH_3\ (c) = +146 \pm 6\ kJ/mol$

$\Delta H_{formation}$ of $NI_3\ (g) = +287 \pm 23\ kJ/mol$

nitrogen–iodine bond energy, E(N–I) = 169 ± 8 kJ/mol

http://chemwiki.ucdavis.edu/Core/Theoretical_Chemistry/Chemical_Bonding/General_Principles_of_Chemical_Bonding/Bond_Energies

N ≡ N bond energy = 941 kJ/mol

I-I bond energy = 149 kJ/mol

Determine Properties from Bond Type (from Chem 1A)

Do Explosives Have Strong Bonds or Weak Bonds?

Which list shows the relative bond *strengths* (strongest to weakest)?

a. single bond > double bond > triple bond

b. triple bond > double bond > single bond

c. double bond > triple bond > single bond

Which bond is easiest to break?

Which bond releases the most energy when formed?

Determine Properties from Bond Type (from Chem 1A)

Do Explosives Have Strong Bonds or Weak Bonds?

Which list shows the relative bond *lengths* (longest to shortest)?

a. single bond > double bond > triple bond

b. triple bond > double bond > single bond

c. double bond > triple bond > single bond