Learning Guide for Chapter 1 - Atoms and Molecules

I. Introduction to Organic Chemistry (1-1)

What will we be studying in organic chemistry?

compounds containing carbon

Why is it called organic chemistry?

the first organic compounds came from living organisms

What did early organic chemists think about organic compounds?

contained a "vital force", couldn't be synthesized

What fields of study does organic chemistry prepare you for?

chemistry, biology, botany, biochemistry, chemical/biomedical engineering, medicine - pharmacy, nutrition, dentistry

What industries depend upon organic chemistry?

pharmaceuticals, petroleum, plastics, agriculture

Why are organic compounds so important?

there are so many - 95% of all known compounds are organic

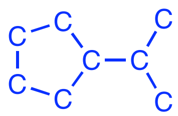
molecules of life are organic - protein, DNA, carbohydrates, fats

Why are there so many organic molecules?

carbon makes 4 bonds - very versatile

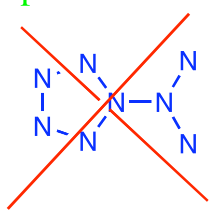
C-C bonds are very stable

C is the only element that makes complex, stable structures

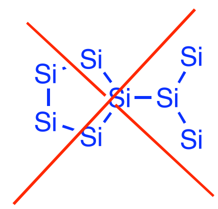


C-C is very stable because it is small,
and has a low electronegativity

(not a complete molecule)



too electronegative



too big

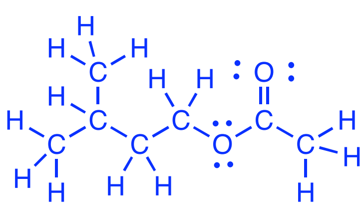
How are organic compounds put together?

framework of C atoms (mostly)

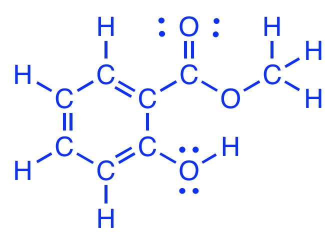
as many H's as needed to fill octet rule

O, N and other atoms in a few stable arrangements

Here are two examples of organic compounds, to give you a preview of the kinds of things we will be working with.



isopentyl acetate
banana flavoring



methyl salicylate
oil of wintergreen

This chapter will review the things you need to know about atoms, ions, and molecules in order to begin our study of organic compounds.

II. Review of Atomic Structure (1-2)

Elementary Particles

What three elementary particles make up an atom? What charge does each have?

electron	proton	neutron
-1	+1	0

Draw a simple picture of an atom, showing how these elementary particles are arranged.

protons/neutrons in the middle, electrons on the outside

What's in the middle of the atom? nucleus

What does the nucleus have in it? protons and neutrons

What is around the nucleus? electrons

Which part participates in chemical reactions? Why? electrons
they're on the outside

Periodic Table of Elements

What is an element? How many of them are found in nature?

element = kind of atom, substances the world is made of

90 naturally occurring

What gives an atom its identity? number of protons = atomic number

What is the atomic number of carbon? six
all carbon atoms have 6 protons
any atom with 6 protons is a carbon atom

How are the elements organized in the Periodic Table?

atomic number goes across, then starts on the next row

Why is the Periodic Table so useful?

you can predict the behavior of an element based on its position on the table

Locate the following on the Periodic Table below:

metals

why are they called this? - properties of elemental substance

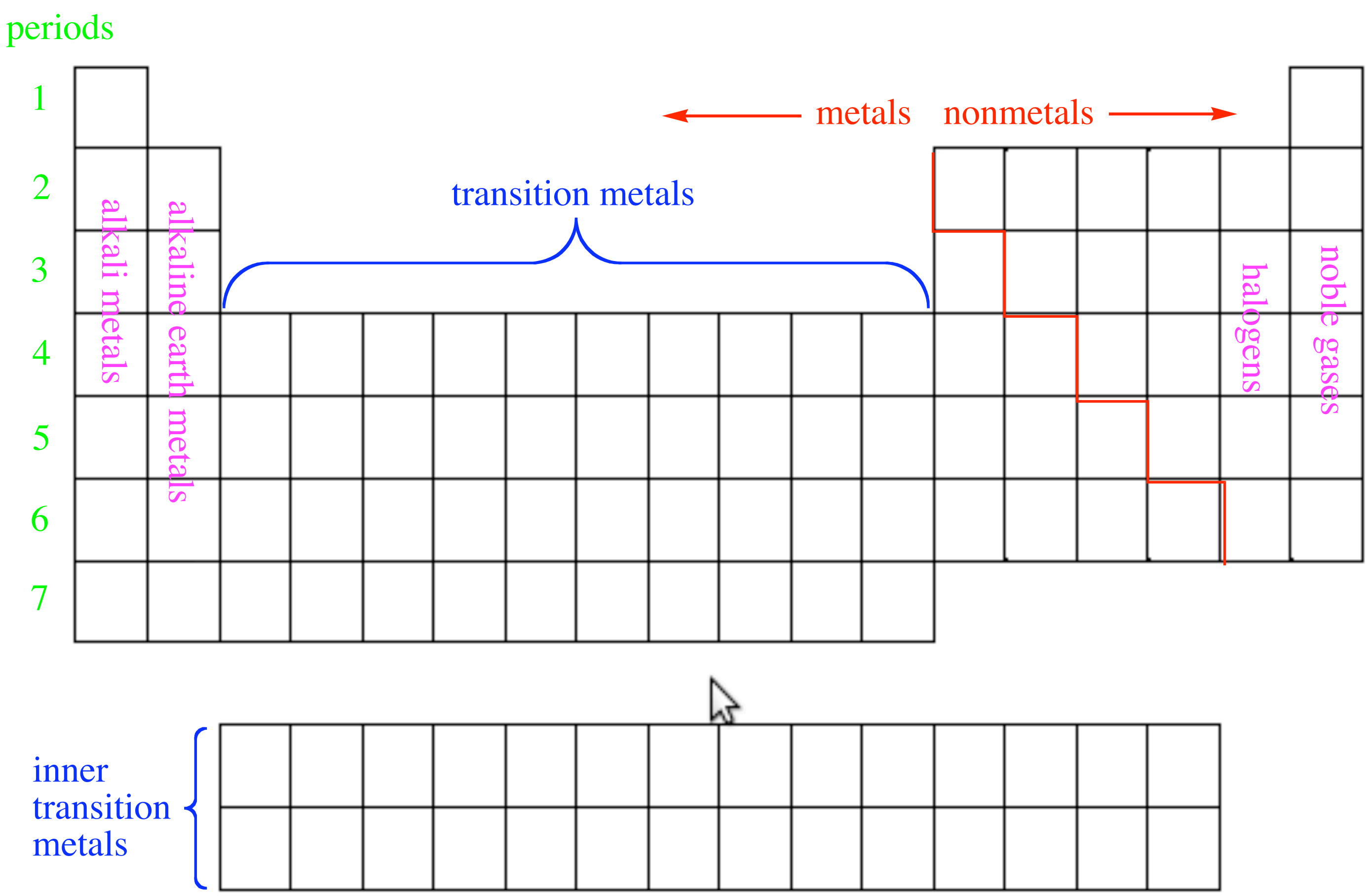
nonmetals

transition metals

inner transition metals

periods 1-7

alkali metals, alkaline earth metals, halogen family, noble gases



What happens to the size of an element as you go across a period? Why?

smaller - but not much (more protons pull electrons closer)
behavior is not affected

What happens to the size of an element as you go down a family? Why?

much larger (new energy level of electrons)
changes the behavior significantly

Where will you find elements with similar chemical reactivity?

in the same family (or group)

Write in the symbols of the following elements in the Periodic Table below:

Four most common elements in organic compounds:

carbon (C)
hydrogen (H)
nitrogen (N)
oxygen (O)

Other nonmetals:

fluorine (F)
chlorine (Cl)
bromine (Br)
iodine (I)
boron (B)
sulfur (S)
phosphorus (P)

Main group metals:

lithium (Li)
sodium (Na)
potassium (K)
magnesium (Mg)
aluminum (Al)

Transition metals:

chromium (Cr)
manganese (Mn)
mercury (Hg)
palladium (Pd)
platinum (Pt)
iron (Fe)
silver (Ag)
zinc (Zn)
copper (Cu)
osmium (Os)

Memorize the positions of these elements (except the transition metals)!
You will need to draw this table from memory.

H																	
Li												B	C	N	O	F	
Na	Mg											Al		P	S	Cl	
K					Cr	Mn	Fe			Cu	Zn					Br	
									Pd	Ag						I	
							Os		Pt		Hg						

What period are carbon, nitrogen, and oxygen in? What about sulfur and phosphorus?

2nd period

3rd period

Which element is in the same family as oxygen? Nitrogen? Boron?

sulfur phosphorus aluminum

Electronegativity

What is electronegativity? ability of an atom to attract electrons towards it

Do nonmetals have high or low electronegativities? What about metals?

high low

What is the most electronegative element? fluorine

Which is more electronegative, nitrogen or oxygen? EN increases →

Which is more electronegative, nitrogen or phosphorus? EN increases ↑

Which of these two comparisons is more important?

N vs O is more important than N vs P

* When considering two elements in the same period, what property is most important?

electronegativity

* When considering two elements in the same family, what property is most important?

size

Atomic mass and isotopes

Which elementary particles contribute the most to the atomic mass? protons and neutrons

What is an isotope? an atom with a specific number of neutrons

What does ^{13}C mean? How else could it be written? How many protons and neutrons does it have?

^{13}C = carbon with a mass of 13

6 protons 13 - 6 = 7 neutrons

How are isotopes useful in organic chemistry?

you can keep track of a certain atom

What is the weighted average of all naturally occurring isotopes of carbon? 12.01

from the Periodic Table

What is the most common isotope of carbon? ^{12}C

(there is about 1% 13C, and a minuscule amount of 14C)

Ions

What elementary particles determine the charge of an atom? protons + electrons -

Which of these is an atom more likely to lose or gain, and why?

lose or gain electrons - they are on the outside of the atom

What happens to an atom when it loses an electron? becomes positive - more p+ (cation)

What happens to an atom when it gains an electron? becomes negative - more e- (anion)

How many electrons would have each element have under the following conditions?

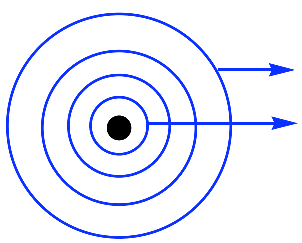
	neutral: same as protons	+1 charge:	-1 charge:	+2 charge:	-2 charge:
fluorine	9	8	10	7	11
calcium	20	19	21	18	22

Which of these ions is most likely to be formed? F^-, Ca^{+2} (fill valence shell)

Which is a cation, and which is an anion? Ca^{+2} cation; F^- anion

Valence Electrons

Draw some circles to represent the energy levels around the nucleus below. Which is the lowest energy? Which is the highest? How do the electrons fill these levels?



electrons go to lowest energy available

Which are the valence electrons? Why are they important?

the electrons in the highest occupied energy level
they're the ones that react, determine the number of bonds an element will form

How many valence electrons do each of the following elements have?

H 1 O 6 Mg 2 F 7 Al 3 P 5

Draw the Lewis dot structures for the following atoms.

III. Review of Ionic and Covalent Bonds

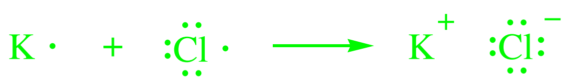
<u>Overview of Ionic and Covalent Bonds</u>

Why do atoms form chemical bonds? to become more stable, fill up valence electrons

What is the octet rule? atoms need 8 electrons in valence energy level to be stable

What kind of compound is KCl? How do you know? Use Lewis structures to show how it would be formed.

ionic - metal and nonmetal (one loses, one gains electrons)



transfer of electrons

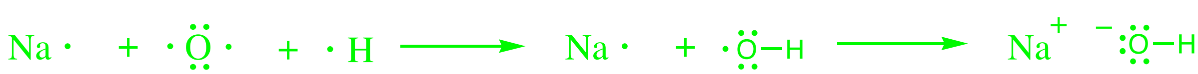
What kind of compound is HCl? How do you know? Use Lewis structures to show how it would be formed.

covalent – two nonmetals (both need electrons, have to share)

sharing electrons

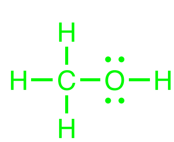
What does a line between two atoms represent? a covalent bond - shared pair of electrons

What kind of bonds does NaOH have? both ionic and covalent



When are covalent bonds found in organic chemistry?

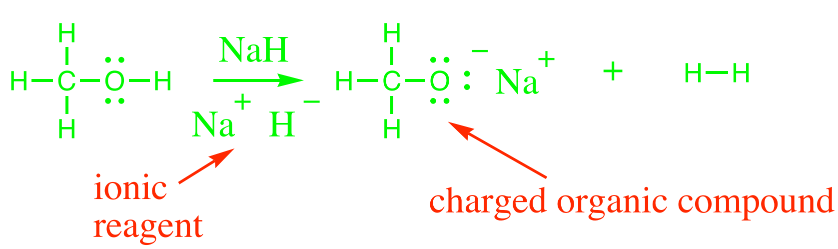
all stable compounds



methanol, a stable compound

When are ionic bonds found in organic chemistry?

compounds may become charged during a chemical reaction
ionic compounds may also be used as reagents



Lewis structures of covalent compounds

What steps should you follow when drawing the Lewis structure of a compound?

1) draw out the atoms with their valence electrons
2) look at how many bonds each one needs to make
3) put atoms together to form bonds
4) make double or triple bonds if necessary

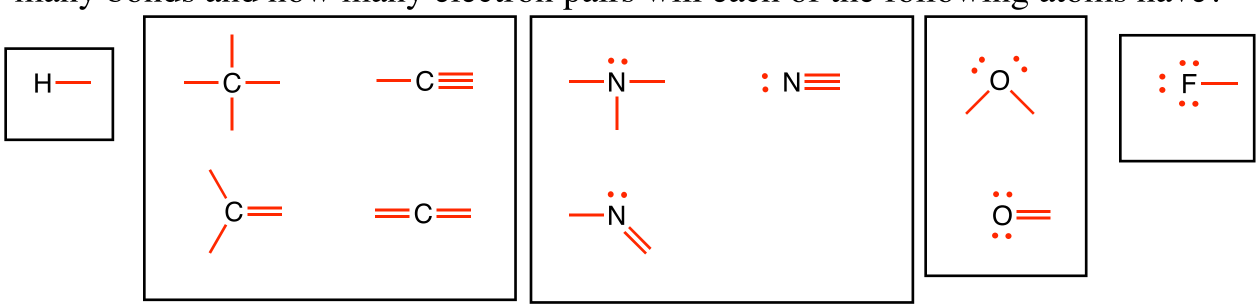
Draw the Lewis structure of each atom below. Then calculate the number of bonds that each atom will typically form.

	H	C	N	O	F
valence electrons	1	4	5	6	7
number of bonds	1	4	3	2	1

What is the relationship between these numbers?

# of unpair e- = # of bonds   add up to 8!

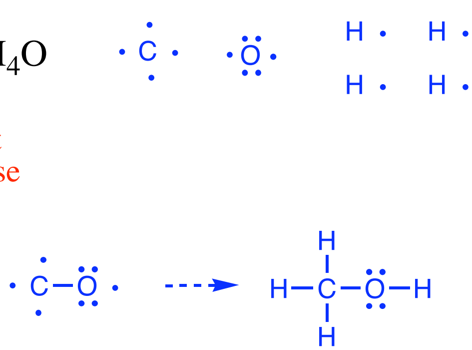
How many bonds and how many electron pairs will each of the following atoms have?



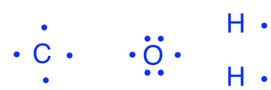
Draw a Lewis structure for the following compounds.

CH_4O

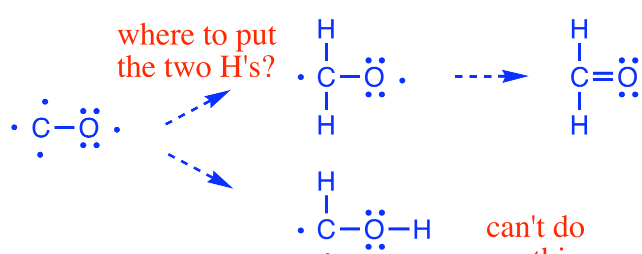
cross out as you use



CH_2O

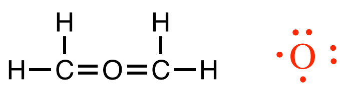


where to put the two H's?

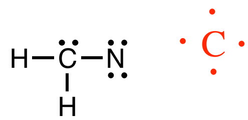


can't do anything

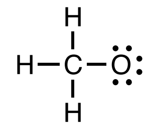
What is wrong with each of the following structures?



O has too many bonds
wrong number of electrons

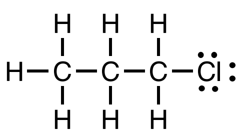


N doesn't fill octet rule
carbon has two many electrons

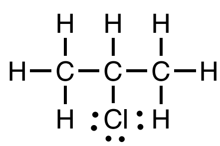


O has too many
electrons

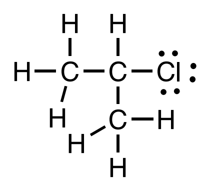
Which of the following structures represent different compounds, and which are just different ways to draw the same compound?



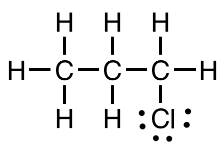
A



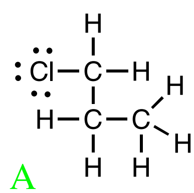
B



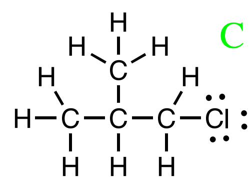
B



A



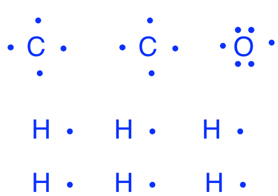
A



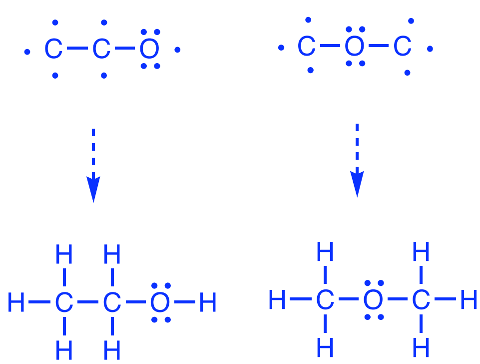
C

Draw two different Lewis structures for each of the following formulas.

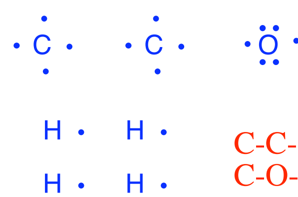
C_2H_6O



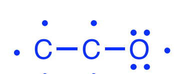
something different?
different arrangement
of original atoms



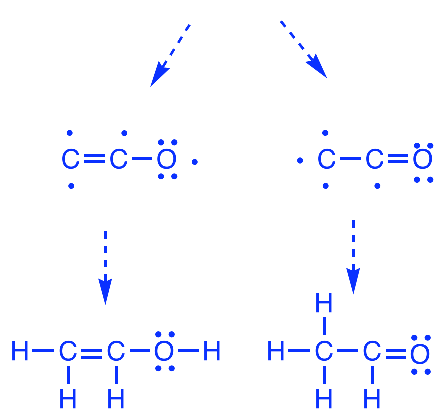
C_2H_4O

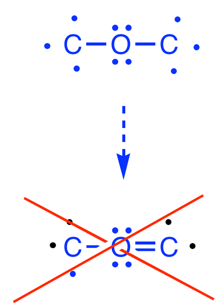


C-C-O or
C-O-C

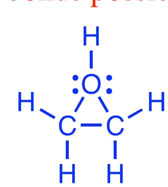


not enough H's;
try double bond





no double
bonds possible!



but you can
make a ring!

Polarity of Covalent Bonds

When are covalent bonds polar? When are they nonpolar?

polar - different electronegativities

nonpolar - same electronegativity

Which atom in a C-F bond is partially positive? Which is partially negative? Why? How can we show this?

δ+ δ -
C—F

C—F

F is more electronegative
becomes partially negative

Describe the polarity of the following bonds and the partial charges on the atoms:

C—C nonpolar, no partial charges

C—H slightly polar, C is slightly negative, H is slightly positive
may be important, may not; may be referred to as nonpolar

C—Cl polar bond, C is partially positive, Cl is partially negative

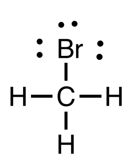
C—Li very polar bond, C is partially negative, Li is partially positive

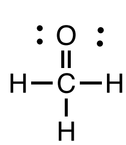
O—H polar bond, O is partially negative, H is partially positive

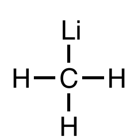
Which is the more polar bond? Why?

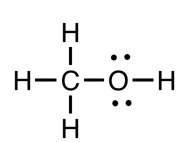
C—N	C—O more polar	O is more electronegative than N
C—O	C=O more polar	multiple bonds are more polar than single bonds (multiple bonds amplify the polarity)
C—H more polar	C—C	H is less electronegative than C (but not by much!)

Locate and label the most important polar bond(s) in each of the following molecules.









Strength of Covalent Bonds

Why is the strength of a bond important?

weak bonds are more reactive - easily broken in a chemical reaction

Predict the trend in the following sequences. Do the bonds get stronger or weaker? Why?

stronger
shorter →

1.	C–C	C=C	C≡C	more bonds = stronger bond	
	83	146	200	bond energy (kcal/mol)	energy it takes to break the bond

weaker
longer →

2.	C–F	C–Cl	C–Br	C–I	larger atoms = weaker bond
	1.41	1.76	1.91	2.10	average bond length
	105	79	66	57	bond energy

stronger →

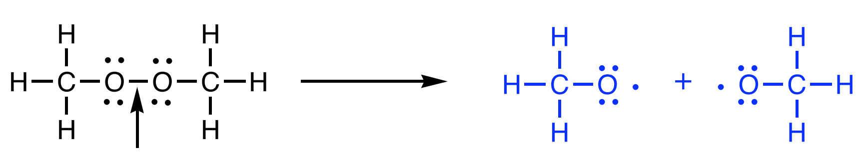
3.	O–O	Cl–Cl	C–C	two electronegative atoms = very weak	
	1.32	2.0	1.54	average bond length	
	33	58	83	bond energy	why is Cl-Cl longer? bigger atoms!

What is the difference between homolytic and heterolytic bond cleavage? Which is more common?

homolytic - both atoms get one of the electrons

heterolytic - more EN atom gets both electrons   more common

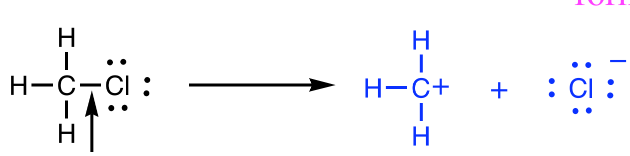
How would the following bonds be likely to break in a reaction?



weakest bond

forms radicals

homolytic - two electronegative atoms bonded



weakest bond

forms ions

heterolytic - atoms of differing electronegativities (more EN atom takes e's) [also, long bond]

Geometry of Molecules

What does the geometry of a molecule tell us about it?

the way the atoms are arranged around a central atom

What principle allows us to predict molecular geometries?

electron pairs will be as far apart as possible

Predict the geometry of an atom surrounded by the following:

4 atoms, no electron pairs – tetrahedral

3 atoms, no electron pairs – trigonal planar

2 atoms, no electron pairs – linear

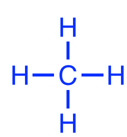
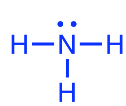
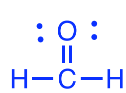
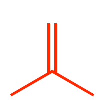
3 atoms, 1 electron pair – trigonal pyramid

2 atoms, 1 electron pair – bent

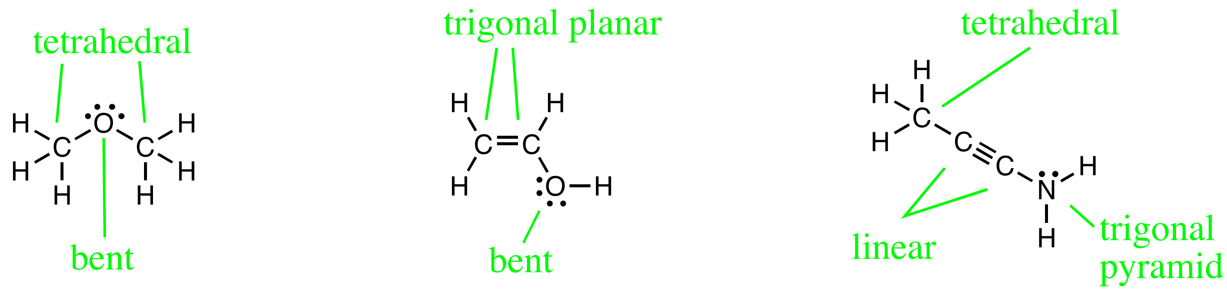
2 atoms, 2 electron pairs – bent

models:
black = carbon or nitrogen
red = oxygen
white = hydrogen
green = halogen
gray tubes = single bonds
white tubes = double or triple bonds

Draw Lewis structures for the following compounds. Then build a model of the molecule and sketch a picture of it. What shape do the atoms surrounding the central atom make? What angle do they make with each other?

	Lewis structure	sketch of model	shape	angle
methane CH_4 (4 atoms, no e- pairs)			tetrahedral	109.5°
ammonia NH_3 (3 atoms, 1 e- pair)			trigonal pyramid	< 109.5°
water H_2O (2 atoms, 2 e- pairs)			bent	< 109.5°
formaldehyde CH_2O (3 atoms, no e- pairs)			trigonal planar	120°
hydrogen cyanide HCN two atoms, no e- pairs)			linear	180°

What is the geometry around each atom in the following compounds?



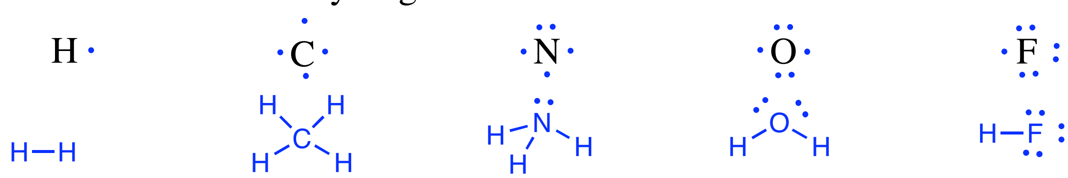
<u>Molecules with charges</u>

What happens when an atom in a covalent molecule loses or gains an electron?

atom becomes charged (the whole molecule is now charged)
an ionic bond is formed

Atoms with no charge:

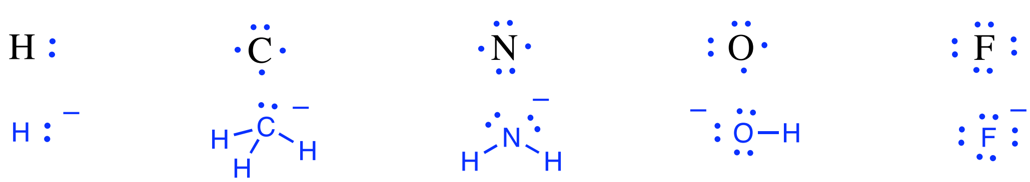
Draw the Lewis structures for the following atoms. What compound would each of them form with hydrogen?



hydrogen gas | methane | ammonia | water | hydrofluoric acid

Atoms with a negative charge:

Draw the Lewis structures for the each of the atoms below if they gained an electron and became negatively charged. What would happen to the compounds they would make?



hydride ion | carbanion | amide ion | hydroxide ion | fluoride ion

Which of the above is the most reactive? Which is the most stable? Why?

electronegativity $F^- > O^- > N^- > C^- \sim H^-$

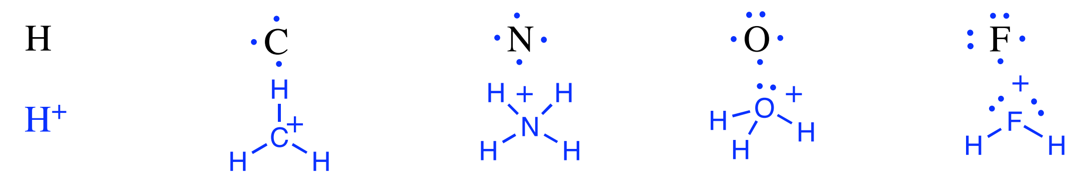
most stable most reactive

Are these molecules more or less reactive than the neutral molecules? more

except maybe F^-

Atoms with a positive charge:

Draw the Lewis structures for each of the atoms below if they lost an electron and became positively charged. What would happen to the compounds they could make?



hydrogen ion carbocation ammonium ion hydronium ion ???

Which of the above are the least stable? Why?

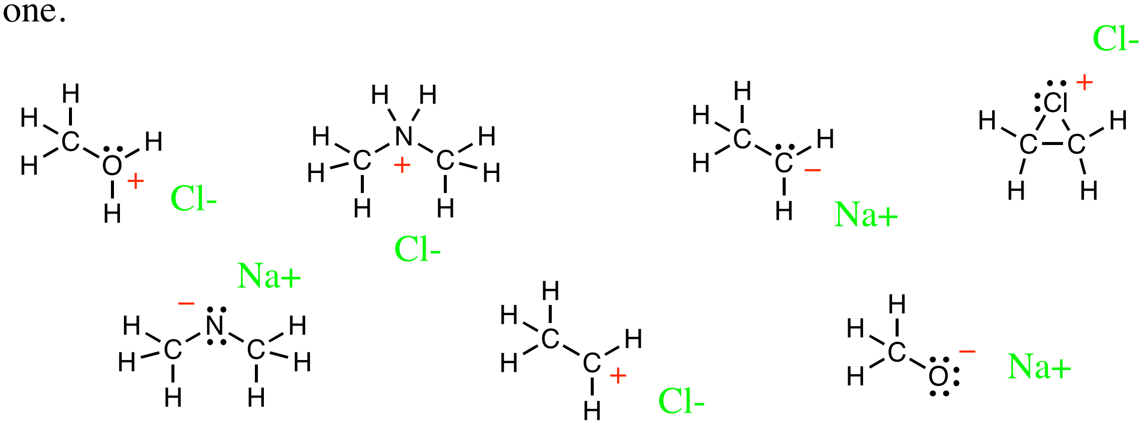
C doesn't have an octet - very reactive

electronegativity $N^+ > O^+ > F^+$

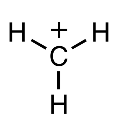
more stable more reactive

H^+ only exists by itself only in the gas phase

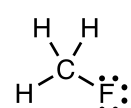
Write in the charges in each of the following compounds. Then draw in a counterion for each one.



What is the difference between the charges on these carbon atoms?

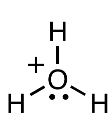


fully charged - ionic
needs a counter ion



partial charge - covalent
contains both charges

Consider hydronium ion (H_3O^+). How can the oxygen be both partially negative and still have a positive charge?



full positive charge - has lost an electron
the polar bonds to the H's lessen the charge on the O, spreading some of it to the H's

Resonance structures

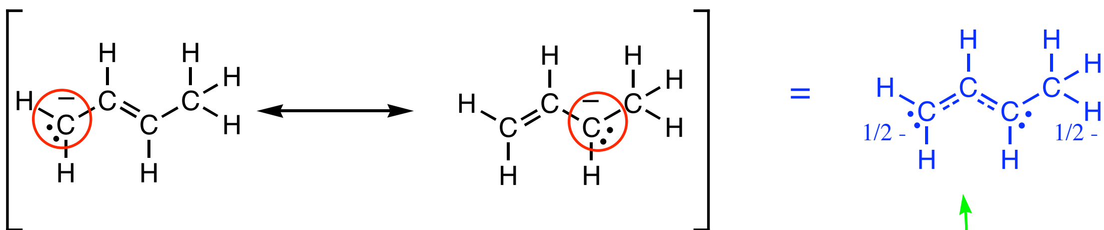
When do molecules have to be represented by resonance structures?

nonbonding electron pairs spread over more than 1 atom
bonds spread over more than 2 atoms

What kinds of molecules typically exhibit this kind of behavior?

molecules with multiple bonds next to charged atoms

Look at the following example:



Where is the double bond? spread across all three C's

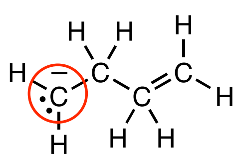
Where is the nonbonding electron pair? shared by the 1st and 3rd C's

What does the compound really look like?

How can we show that these are resonance structures?

[ ] , ⟷

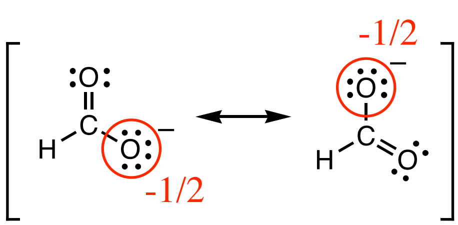
The following molecule does not have any resonance structures. Is it more or less stable than the one above?



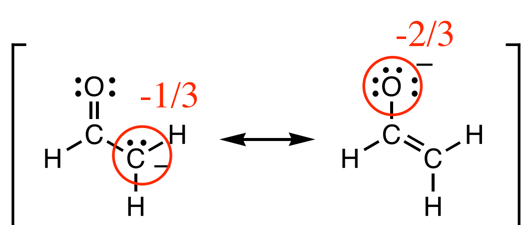
less stable - no resonance, charge concentrated on one atom

compound above has 2 resonance structures - charge is spread out

Which of the following resonance structures have equal resonance contributors, and which have unequal resonance contributors? Why?



equal resonance contributors
negative charge shared by 2 O's



C^- vs. O^-

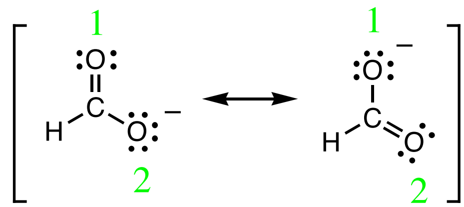
lesser resonance contributor

greater resonance contributor

Why are the molecules below the same, but the resonance structures different?

2 identical molecules

free to rotate

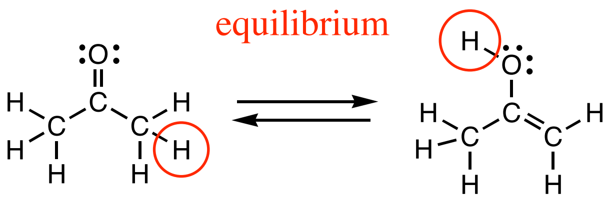


1 molecule

not free to rotate - O in one position must correspond to the other.

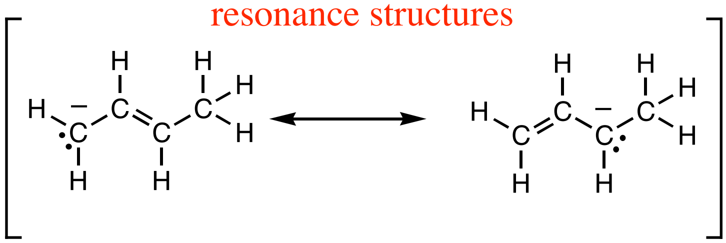
How is a resonance structure different from two molecules in equilibrium?

equilibrium



something is happening
2 different molecules exist
bonds are broken and formed
* an atom is in a different place

resonance structures



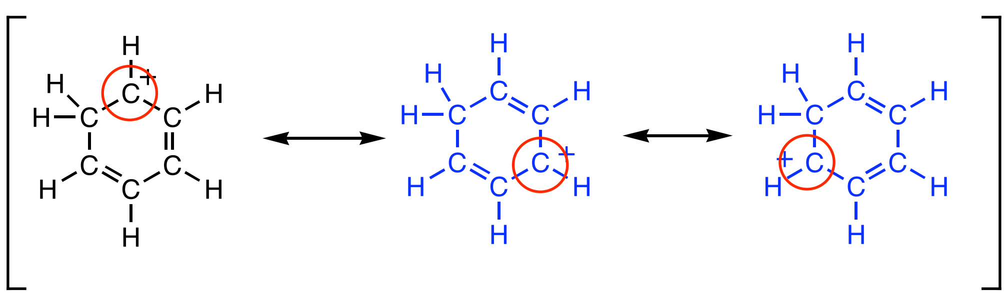
nothing is happening
only 1 molecules exists
electrons spread around
* all atoms in the same place

How can you tell which is which?

equilibrium atoms are in different places $\rightleftharpoons$

resonance - atoms in the same places [$\longleftrightarrow$]

Fill in the missing resonance structures.



Why is this carbocation unusually stable? positive charge spread over 3 C's

IV. Orbitals and Hybridization

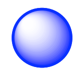
Atomic orbitals

What is an atomic orbital? place where a pair of electrons can be
(space where the probability of finding an electron is high)

How many electrons can fit into one atomic orbital? 2

What are the four kinds of atomic orbitals? s, p, d, f

How many of each type of orbital are found? s - 1; p - 3; d - 5; f - 7

What shapes do the first two orbitals have? s - spherical  p - dumbbell 

What orbitals are present in which in which energy levels?

1 - s 2 - s, p, p, p 3 - s, p, p, p, d, d, d, d, d 4 and up - s, p, p, p, d, d, d, d, d, f, f, f, f, f, f, f

Give the electron configuration for each of the following atoms:

H $1s^1$ H only has an s orbital with an electron

C $1s^2\ 2s^2 2p^2$

N $1s^2\ 2s^2 2p^3$ C, N, O have s and p orbitals with e-

O $1s^2\ 2s^2 2p^4$

P $1s^2\ 2s^2 2p^6\ 3s^2 3p^3$ P, S have s and p orbitals with e-, empty 3d orbital

Molecular orbitals

What is a molecular orbital? joins 2 nuclei - a covalent bond

Where do molecular orbitals come from? joining atomic orbitals

How many electrons can fit into one molecular orbital? two

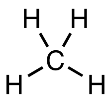
What are the two kinds of molecular orbitals? sigma σ pi π

What are the two kinds of covalent bonds? sigma σ pi π

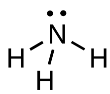
Which bonds in a molecule are sigma bonds? all single bonds
1st bond of double and triple bonds

Which bonds in a molecule are pi bonds? 2nd bond of double bonds,
2nd and 3rd bond of triple bonds

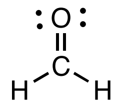
Label the bonds in the following molecules.



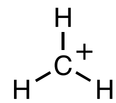
4 sigma's



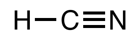
3 sigma's



3 sigma, 1 pi

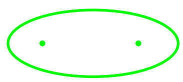


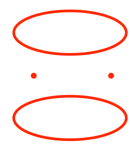
3 sigma's



2 sigma, 2 pi

What does a sigma bonding orbital look like? What does a pi bonding orbital look like?

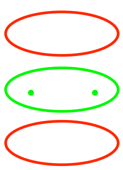
sigma: a fat sausage 

pi: a hot dog bun 

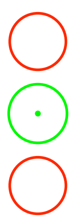
Why are pi bonding orbitals needed when forming a double or triple bond?

so that two or three bonds can fit between two atoms
(orbitals can't occupy the same space)

double bond:

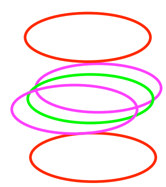


from the side

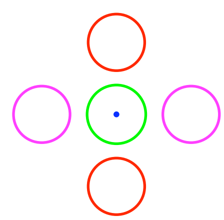


from the end

triple bond:



from the side

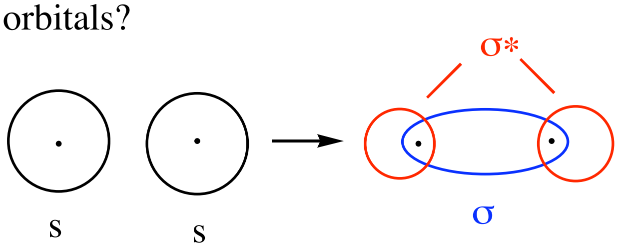


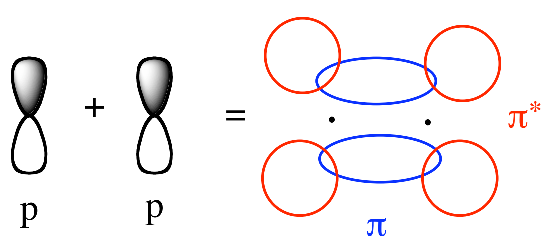
from the end

When a sigma or pi bonding orbital is formed, what other kind of orbital is also formed?

antibonding orbital sigma-star, pi-star

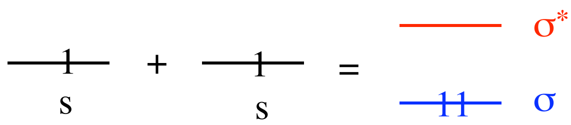
How is a sigma orbital formed from two s orbitals? How are pi orbitals formed from two p orbitals?

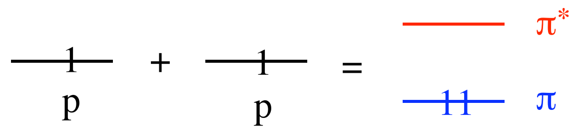




Why are antibonding orbitals called this? if occupied, they pull the atoms apart instead of holding them together

Draw lines representing the energy of the sigma bonding, sigma antibonding, pi bonding, and antibonding orbitals in the following diagrams.





Which is more stable, an atomic orbital or a molecular bonding orbital?

bonding orbitals are lower in energy = more stable

Why are the antibonding orbitals usually empty?

the electrons go to the lower energy orbitals

Which is likely to be more reactive, electrons in a sigma bonding orbital or a pi bonding orbital?

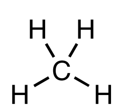
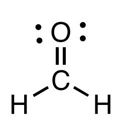
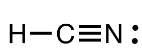
pi bonding orbital; higher energy = more reactive

lower energy = more stable = less reactive

higher energy = less stable = more reactive

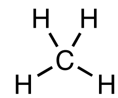
Hybridized atomic orbitals

What problem do we find when trying to form molecular orbitals for the following molecules?

	molecular orbitals	atomic orbitals	hybrid orbitals
	σ σ σ σ	H: s C: s p p p	sp^3 sp^3 sp^3 sp^3
	σ σ σ π	H: s C: s p p p	sp^2 sp^2 sp^2 p
	σ σ π π	H: s C: s p p p	sp sp p p

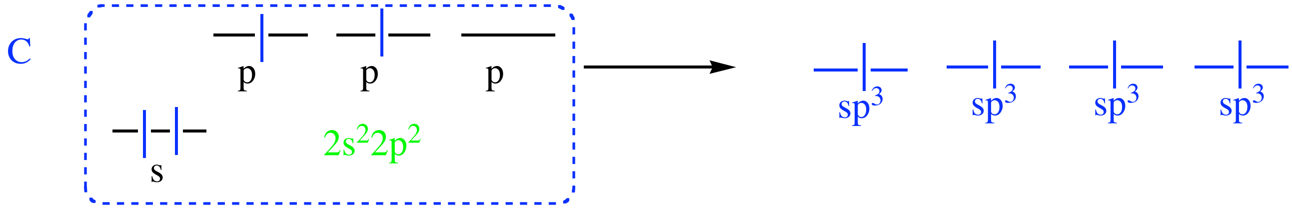
Problem: we don't have enough s orbitals to make the necessary number of sigma bonds

Solution: mix the atomic orbitals together to make hybrid orbitals

How many hybrid orbitals does methane need?  4; all sigma bonds

What hybridization will it have? sp^3

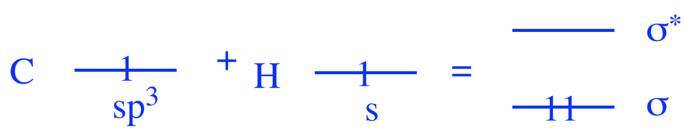
atomic orbitals | hybridized atomic orbitals

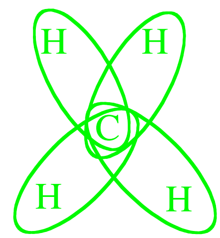


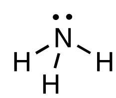
What do sp^3 orbitals look like? skinniest

How are they oriented? tetrahedral model of four tetrahedral orbitals

How will each of the bonds be formed?

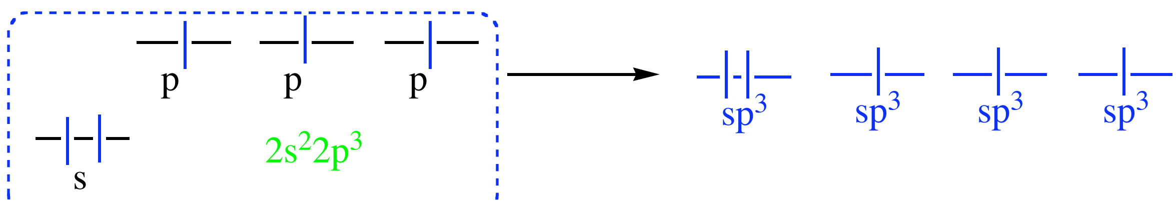




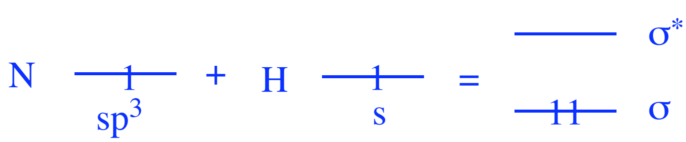
How many hybrid orbitals does ammonia need? 

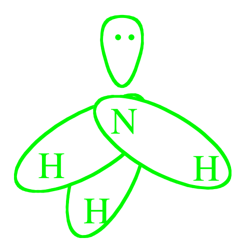
4 - nonbonding pair goes in a hybrid orbital so it can spread out

What hybridization will it have? sp^3

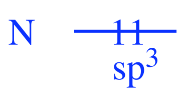


How will each of the bonds be formed?



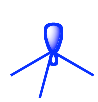


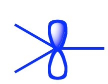
Where will the lone pair go?



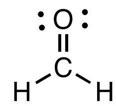
How do we know it doesn't stay in a p orbital? it has a choice - sp^3 is more stable

geometry


sp^3 orbital
trigonal pyramid


p orbital
trigonal planar

How many hybrid orbitals does formaldehyde need?



O: 1 sigma, 1 pi, 2 e- pairs
C: 3 sigma's, 1 pi

C and O both need 3 - both need to make one pi bond

What hybridization will they have? sp^2

C: s ($\uparrow\downarrow$), p ($\uparrow$), p ($\uparrow$), p ( ) $\longrightarrow$ sp^2 ($\uparrow$), sp^2 ($\uparrow$), sp^2 ($\uparrow$), p ($\uparrow$)

O: s ($\uparrow\downarrow$), p ($\uparrow\downarrow$), p ($\uparrow$), p ($\uparrow$) $\longrightarrow$ sp^2 ($\uparrow\downarrow$), sp^2 ($\uparrow\downarrow$), sp^2 ($\uparrow$), p ($\uparrow$)

What do sp^2 orbitals look like? a bit fatter

How are they oriented? trigonal planar, w/ p orbital up and down
model of three trig planar, one p

How will the C-H bonds be formed?

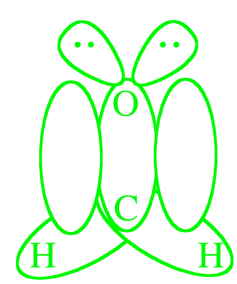
C sp^2 ($\uparrow$) + H s ($\uparrow$) = σ^* ( ), σ ($\uparrow\downarrow$)

How will the C-O sigma bond be formed?

C sp^2 ($\uparrow$) + O sp^2 ($\uparrow$) = σ^* ( ), σ ($\uparrow\downarrow$)

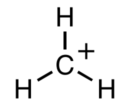
How will the C-O pi bond be formed?

C p ($\uparrow$) + O p ($\uparrow$) = π^* ( ), π ($\uparrow\downarrow$)



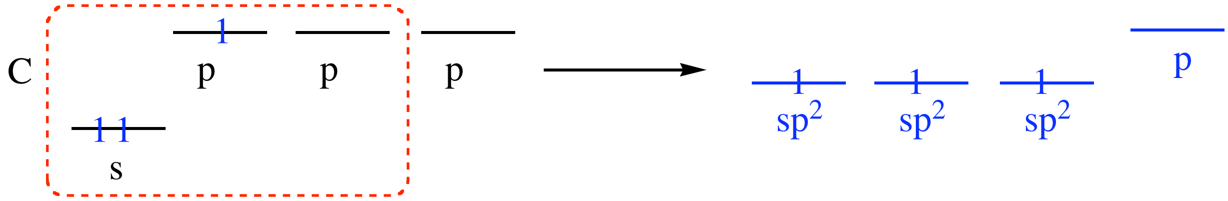
Where will the two lone pairs go?

O sp^2 ($\uparrow\downarrow$) O sp^2 ($\uparrow\downarrow$)

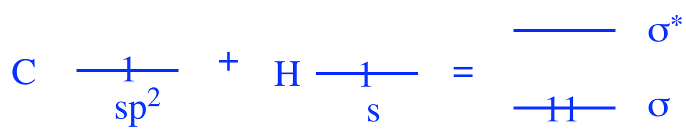
How many hybrid orbitals does a methyl cation need? 

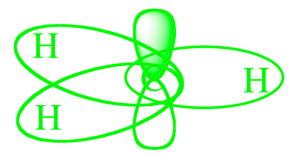
only 3 - the empty orbital will be a p orbital

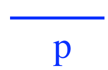
What hybridization will they have? sp^2



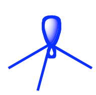
How will the C-H bonds be formed?

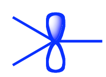


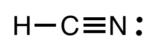


Where is the positive charge? 

Why is the empty orbital a p orbital? it has a choice - p is more stable

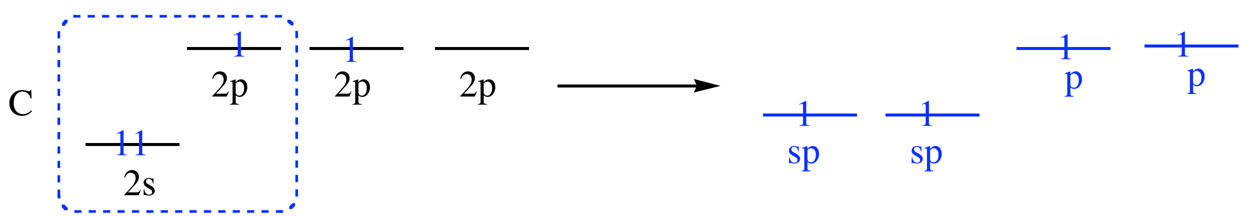
geometry  sp^3 orbital
trigonal pyramid

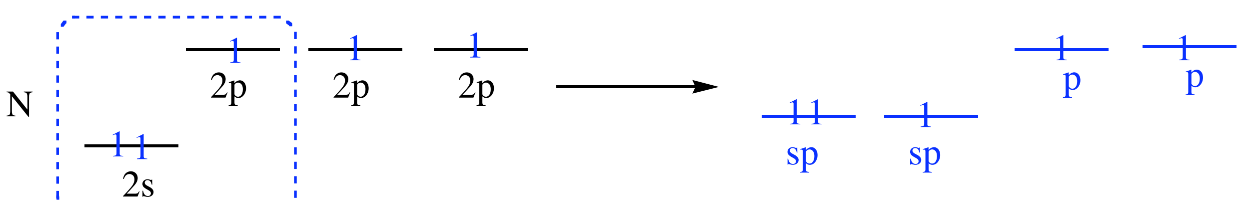
 p orbital
trigonal planar

How many hybrid orbitals does hydrogen cyanide need? 

only 2 - two sigma bonds and two pi bonds

What hybridization will they have? sp

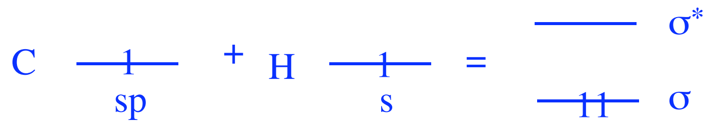




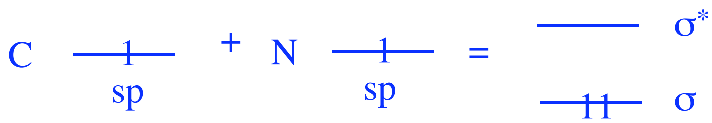
What do sp orbitals look like? fattest model of two sp, two p

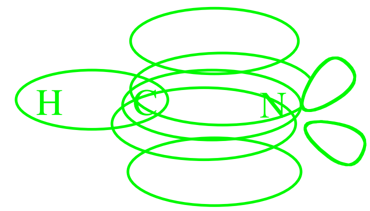
How are they oriented? linear, w/ two p orbitals on other axes

How will the C-H bond be formed?

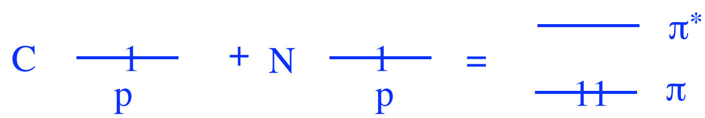


How will the C-N sigma bond be formed?

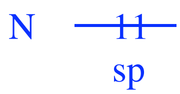




How will the two C-N pi bonds be formed?

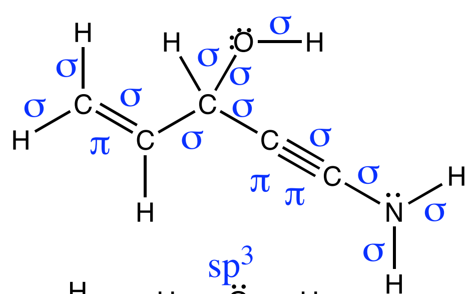


Where is that nonbonding electron pair?

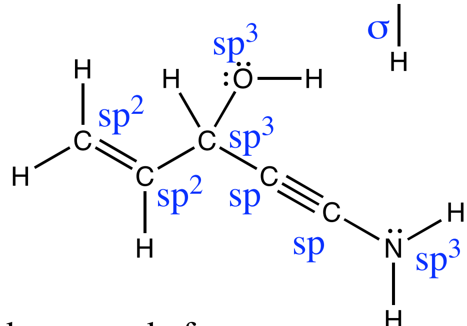


Putting it all together:

Label all bonds as sigma or pi bonds.



Label the hybridization of each atom.



Label the atomic orbitals that each bond was made from.